

FY 2001 ANNUAL OPERATING PLAN

HYDROGEN PROGRAM

Prepared for

**U. S. DEPARTMENT OF ENERGY
OFFICE OF POWER TECHNOLOGIES**

by

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1.0 INTRODUCTION

This document is the Annual Operating Plan of the Department of Energy (DOE), Hydrogen Research and Development (R&D) Program. It serves to provide the DOE's management and program participants with the plans for fiscal year 2001 (FY 2001). This document contains general information on the Hydrogen R&D Program and its goals, project summaries listing the planned activities for FY 2001 (including Gantt charts with expected critical and key milestones), significant results and accomplishments from 2000, and listings of publications, patents, and national recognition achieved by the Principal Investigators.

The Hydrogen Program is part of the Office of Power Delivery Systems within the Office of Power Technologies (OPT), which is in turn within the Office of Energy Efficiency and Renewable Energy. The organization of the Hydrogen Program is detailed in Chapter 2. The Program includes three focus areas: A) Research and Development of Critical Component Technologies (production, storage, and utilization), B) Technology Validation, and C) Analysis and Outreach.

The DOE Hydrogen R&D Program supports the Matsunaga Hydrogen Research, Development, and Demonstration Act of 1990 (P.L. 101-566), the Energy Policy Act of 1992 (P.L. 102-486) Section 2026, and the Hydrogen Future Act of 1996 (P.L. 104-271), and addresses the energy and environmental benefits of hydrogen. The Program put forth by the DOE, in collaboration with industry and other Federal entities, has been designed to develop the technologies necessary to safely produce, store, transport, and utilize hydrogen as an energy carrier; to illustrate the energy and environmental benefits to the public sector; and to initiate the transition strategy which can bring these technologies successfully to the marketplace.

1.1 Implementing the Twenty-Year Vision

Hydrogen allows for both the increased use of renewable energy and CO₂ sequestration technologies that help to reduce CO₂ emissions. It can replace conventional fuels and result in near-zero urban pollutants being emitted into the atmosphere. With this in mind, the DOE Hydrogen program laid out its Twenty-Year Vision in the Strategic Plan:

In the next twenty years, concerns about global climate change and energy security will create the platform for the penetration of hydrogen into several niche markets. Ultimately, hydrogen and electricity will come from sustainable renewable energy resources, but fossil fuels will be a significant transitional resource during this period. The growth of fuel cell technology will provide a base for the establishment of the hydrogen option into both transportation and electricity supply markets.

Since the strategic plan was written in 1998, the Hydrogen Program has acted as a catalysts to advance hydrogen technologies. The Twenty-Year vision given in the document was aimed towards the long-term development of renewable based hydrogen technologies. In the interim, fossil fuels are to be a transitional resource. This is significant, because the technologies that use fossil fuels and that enable hydrogen in both the fuel infrastructure and vehicle technologies exist today, and can meet near term markets. Furthermore, as noted by industry participants in a hydrogen blueprint meeting in Sacramento, California, there are **no technical showstoppers** to implementing a near-term hydrogen fuel infrastructure for direct hydrogen fuel cell vehicles. Fundamentally, the technologies required are available but there are engineering development needs as well as codes and standards and other institutional issues to resolve.

A key driver for hydrogen vehicles is the California Zero Emissions Vehicle (ZEV) mandate. The ZEV mandate requires that by the year 2005, 10% of the total vehicles sold will be zero emission vehicles. Under the mandate, the number of “pure ZEVs” (i.e., hydrogen fuel cell vehicles or battery electric vehicles) will be 1% of the total vehicle market or about 10,000 hydrogen fuel cell vehicles.

In the near term, fuel cell vehicles will most likely be used in fleet applications to accommodate higher vehicle costs as well as fueling, operation, and maintenance requirements. Hydrogen-fueled buses will also be utilized in a few urban areas and as well as by some very progressive transit agencies that have compressed natural gas (CNG) fueling facilities. Under the federal Energy Policy Act (EPACT), alternative fuel vehicles (AFV) fleets may provide the most direct opportunities in the near-term. DOE’s overall mission is to replace 30% of petroleum-based motor fuels by the year 2010. EPACT mandates federal, state, and alternative fuel provider fleets to purchase AFVs.

1.2 DOE Hydrogen Program Strategic Approach

The DOE Hydrogen Research and Development Program's mission is to conduct research and engineering development in the areas of hydrogen production, storage, and utilization for the purpose of making hydrogen a cost-effective energy carrier for utility, buildings, and transportation applications. The program is being positioned to support the introduction of hydrogen technologies to meet California’s ZEV mandate requirements, and the push for Distributed Generation.

The program is expanding the short-term applications of hydrogen through partnerships with industry that will allow improvements in efficiency, decrease emissions, and lower the cost of hydrogen production. Projects are being undertaken with fuel cell manufacturers to develop hydrogen based electricity storage and generation systems that will enhance the introduction and production of distributed systems. The program also aims to develop codes and standards and safe systems to facilitate the creation of a hydrogen infrastructure. Systems will be developed that are cost-effective and safe for use in hydrogen vehicles in urban non-attainment areas, in addition to the creation of on-board hydrogen storage systems. The program also aims to lower the cost of technologies that produce hydrogen directly from sunlight and water.

1.2.1 Production Goals

If fuel cell vehicles are going to be competitive on the open market, an infrastructure for the generation and distribution of hydrogen must be established. To compete with other energy carriers, such as electricity, natural gas, and petroleum, the cost of generating hydrogen must come down. A system for distributing the fuel must also be commercially available.

- **Improving the efficiency and lowering the cost of fossil based and biomass-based hydrogen production processes to \$6-\$8/ MMBtu**

Initially, hydrogen utilized in fuel cells will be produced from natural gas. The competing option will be to burn the natural gas/hydrogen blends in combustion turbines or internal combustion engines. To make fuel cells competitive with respect to the combustion options, the cost differential between hydrogen and natural gas must be minimized. Toward this aim, the goal of \$6-\$8/ MMBtu production cost of fossil-based and biomass-based hydrogen was established. In addition, in order to support the transportation market, the Program has set a goal of \$12-\$15/ MMBtu (which is approximately 60-75 cents per gallon of gasoline before taxes, based on a fuel-cell vehicle with an equivalent of about 82mpg) for the cost of producing pressurized hydrogen at the refueling station.

Hydrogen can also be produced by the gasification of dedicated biomass crops for approximately \$6-\$8/ MMBtu. By adding CO₂ sequestration, both the natural gas and biomass strategies can be augmented.

Hydrogen can be produced by these technologies and delivered to a vehicle less expensively than gasoline on a mile per gallon equivalent basis when compared with today's 28 miles per gallon efficiencies.

- **Advancing emission-free and renewable-based hydrogen production technologies towards commercial viability, with a target cost of \$10-\$15/ MMBtu**

In order to advance the mission relating to technologies that produce hydrogen from sunlight and water, the Hydrogen Program will pursue long-term electrolytic, photoelectrochemical, and photobiological research and development. The program has set a goal of producing electrolyzers at efficiencies greater than 92% for less than \$300/ kW.

1.2.2 Storage and Utilization Goals

Hydrogen vehicles will not be cost effective unless storage is priced competitively. Market forces, particularly cost, will be the key driver bringing fuel cell vehicles to compliance with California's ZEV mandate. To facilitate the development of a hydrogen infrastructure to support fuel cell vehicles and ultimately electricity generation from hydrogen, the goals below were developed.

- **Demonstrating safe and cost-effective storage systems for use in stationary distributed electricity generation applications, and for on-board and stationary applications in urban non-attainment areas**

A major improvement in hydrogen storage performance will be necessary for hydrogen to gain acceptance as an effective energy carrier. With intensive interest in mobile applications and as the amount of intermittent renewable electricity increases, hydrogen storage becomes an essential element of these systems. Current technology permits the physical storage, transport, and delivery of hydrogen, in gaseous or liquid form, in tanks and pipeline systems. These physical storage systems have been used in various stationary and mobile demonstrations, but the issues of safety and energy consumption require the development of advanced storage concepts based on advanced materials for physical storage and chemical storage mediums. The program aims to develop storage that will deliver greater than 5% hydrogen by weight at temperatures less than 110°C, for on-board vehicle storage.

- **Developing fuel cell and reversible fuel cell technologies as an efficient low-cost means of converting hydrogen into electric power**

In order to develop a hydrogen infrastructure, the end-use technologies must be developed and matured. Here, the primary technology is the fuel cell. In order for fuel cells to be the "work horse" hydrogen utilization tool, several technical hurdles must be overcome. Fuel cells must be run on hydrogen directly to prevent CO₂ emissions; fuel cell efficiencies must be increased and their cost must be lowered to make them competitive; and reversibly electrolyzer/fuel cell modules must be developed that can enable substantial reductions in overall system costs. The Program aims to produce PEM fuel cells for niche applications, such as small battery replacements that cost less than \$300/kW. In addition, the Program is striving toward reversible fuel cells having a round-trip efficiency of 70%, and a cost of less than \$600/kW.

1.2.3 Technology Validation Goals

This focus area concentrates on validating nearer term technologies against a series of cost, performance, and safety objectives. This can include the integration of any combination of production, storage, transport, and utilization technologies, and is performed in collaboration with industry. These projects will help to facilitate hydrogen technologies' establishment as a viable application and ensure competitiveness with other technologies. Through the Technology Validation Program, DOE's Hydrogen

Program will promote direct hydrogen fuel cell vehicles that meet the demands of California's ZEV mandate.

- **The goal of the Technology Validation is to support industry in the verification and demonstration of hydrogen systems in the utility and transportation sectors.**

Technology validation projects integrate components of novel and advanced technology into test-bed energy systems to evaluate their potential. Parallel development of advanced fossil-based and renewable-based production systems, as well as current and advanced storage and utilization technologies, will provide a set of critical experiences to industry as they evaluate the introduction of the technologies into niche markets.

The strategy of the technology validation is within the Technology Validation Plan. The Program will achieve its goals by operating under the following objectives:

1. Obtain industry participation through competitive solicitations for mid-term development and proof-of-concept testing
2. Integrate renewable energy resources with hydrogen storage in remote, distributed power scenarios
3. Test the viability of hydrogen production, storage, and refueling stations
4. Test the viability of hydrogen production, storage, and refueling stations within several clean clusters
5. Evaluate remote and residential "total" energy PEM fuel cell systems
6. Develop hydrogen-based operating experience acceptable to meet safety codes and standards.

1.2.4 Environmental Goals

The generation and consumption of energy is the largest single source of air pollution in the United States. Electricity produced from fossil fuels results in one-third of all carbon-based emissions. The oil-dependent transportation sector contributes another third. To cut emissions and reduce the effects of harmful urban pollutants, such as NO_x, SO_x, and CO, there must be a shift away from fossil fuel-based energy and an increasing dependence on renewable sources of energy. In response, the Hydrogen Program has set forth the goals of reducing emissions in urban non-attainment areas, and reducing global greenhouse gas emissions. The goals are to displace 1.9 million tons of carbon by 2010 and 13.5 million tons of carbon by 2020. Emissions are to be reduced by 52,000 tons/year of NO_x, 390,000 tons/year of CO, and 45.6 million tons/year of CO₂ by 2020.

1.2.5 Policy, Planning, and Analysis Goals

Analysis and technology transfer incorporates many of the activities formerly grouped under the titles of Systems Analysis and Integration, Technology Transfer, and Industry and Educational Outreach. This includes the identification and definition of research opportunities for hydrogen as an energy carrier through system and infrastructure evaluations and analyses. Analysis will be used to determine the economic feasibility of various scenarios through the calculation of life cycle costs of individual production, storage, transport, and end-use technologies, as well as overall systems. Projects such as technical brochures, fact sheets, and exhibits will all be evaluated and presented to the Program. As set forth in the Strategic Plan the goals of Policy, Planning, and Analysis include:

- **Ensuring that Federal R&D investments in hydrogen production, storage, distribution, and end-use technologies will provide the maximum value added to national strategic goals including global greenhouse emission mitigation**

The goal of supplying significant amounts of renewable hydrogen to the electricity supply and transportation markets in 20 to 30 years cannot be achieved with current budgets unless they are highly leveraged with other Federal programs and with industry. The key planning and analysis issue for the Program is how to define and maximize its "value-added" to the national and global transition to renewable energy.

- **Identifying and evaluating key market segments and market entry conditions for hydrogen utilization in transportation and in electricity generation at distributed and remote locations**

In order for policy makers to make rational decisions regarding the utilization of hydrogen, it is necessary that they receive the pertinent information and recommendations from the Program and industry. These recommendations must evolve from data developed from the development and validation components of the Program, and must incorporate reasonable and thorough systems analysis of hydrogen integrated pathways.

- **Developing and applying metrics to measure the Program's contribution to attaining national strategic energy goals and market share in key segments**

It is necessary for the program to develop a database that will incorporate cost, performance, reliability, lifetime, and other key characteristics for hydrogen technologies to contribute to national strategic energy objectives and compete in key market segments.

1.2.6 Outreach and Coordination Goals

In California, the public must also be aware of the air quality improvements that result from the use fuel cell vehicles and the ZEV mandate. The Program conducts various industry outreach, public outreach, and international activities including efforts in three major areas: workshops and conferences, exhibits and trade shows, and publications. These outreach and technology transfer activities span the entire program structure. The goal of the outreach is:

- **Conduct outreach and coordination to develop informed constituencies in the industrial and public sectors as part of a strategy to accelerate the commercialization of renewable hydrogen technologies.**

For hydrogen to act as an energy carrier, the public must be informed of the technology. The public must be made aware of the economic and environmental benefits of hydrogen technologies, the level of safety associated with hydrogen technologies, and industry's impressive safety record producing and using large quantities of hydrogen.

2.0 TECHNICAL ORGANIZATION

2.1 Approach

The techniques employed by the emphasize state-of-the-art methods for: (1) genetic engineering to develop biological systems that can produce hydrogen directly from water or carbon-rich substrates such as the syngas produced from gasification of biomass; (2) engineering and manufacturing of high performance semiconductors that will directly convert photons (light energy) to hydrogen by splitting water; (3) developing newer high-efficiency methods to thermally break down fossil feed stocks and biomass to produce high purity hydrogen; and (4) producing engineered materials for high performance storage systems such as carbon nanotubes and fullerenes that can adsorb large volumes of hydrogen.

2.2 Objectives

The objectives of the Hydrogen Program are to develop the critical technologies for hydrogen systems and support a vision of a sustainable energy future that includes hydrogen and electricity as the energy carriers. The accomplishment of these objectives will lead to improved energy use and efficiency, lower environmental emissions, and fuel use flexibility.

The Program supports the following activities: (1) developing and integrating the technology base for producing hydrogen using fossil and renewable sources; (2) developing advanced material and delivery systems for storage and transport options; (3) evaluating safety and reliability issues associated with utilization technologies; (4) performing technical and economic analyses on component technologies and processes; and (5) demonstrating hydrogen technologies within integrated energy systems, with strong industry collaboration.

2.3 Management Structure

The Hydrogen Program is managed by the Department of Energy, with technical oversight and management assistance provided by its technical management group; National Renewable Energy Laboratory (NREL), Sandia National Laboratories (SNL) and Los Alamos National Laboratories (LANL). DOE provides technical and programmatic guidance, sets budgetary marks and establishes programmatic goals. The Program organization is shown in Figure 2.1. Headquarters activities are led by the Hydrogen Program Management Team.

The DOE Golden Field Office is responsible for coordination of the Program's cost-shared collaborative agreements. This includes project and financial management, and the issuing, coordinating, and evaluating of the Hydrogen Program's solicitations.

A group of technical managers, made up of scientists and engineers within the program also provide technical guidance and coordinate within the areas of thermal production, photoelectrolytic and photobiological production, storage, and utilization R&D.

The management team is involved with the planning efforts through technical reviews of proposals, annual peer review, and strategic planning meetings. Additionally, the NREL Program Office plans and executes the HTAP meetings, and produces and distributes all publications associated with the Panel and its subcommittees and reviews all production projects. SNL manages those validation projects for remote

power applications, and reviews all storage projects and hydride development and LANL is conducting research on fuel cells.

HTAP, as mandated by the Matsunaga Act and amended by the Hydrogen Future Act, advises DOE management in carrying out the Program. The Panel members, nominated by the Secretary of Energy, represent industry, universities, financial and environmental organizations, and address issues such as developing market-sensitive transition paths from near-term to longer-term programmatic objectives.

The National Hydrogen Association (NHA), which is comprised of industry members, leads the DOE's activities in the development and promulgation of codes and standards related to the safe use of hydrogen. Widespread hydrogen use will require that safety be intrinsic to all processes and systems to ensure the public's complete confidence in hydrogen as a fuel. NHA has taken a lead role in writing new standards through the International Standards Organization, Technical Committee 197, to push forward standards for the safe handling of hydrogen. In addition, DOE has funded a consultant to support the NHA to promulgate new building codes in the United States. This consultant is an expert in working with the International Code Council (ICC). At his request, the ICC created an Ad Hoc Committee (AHC) on hydrogen technologies. This group is supported by the Hydrogen Program through funded experts conducting applied research and development in areas of interest. The AHC is reviewing all of the existing building codes for portable and vehicular fuel cells using hydrogen as a fuel and will recommend to the full ICC any modifications or additions that are required to introduce these technologies into the marketplace.

2.4 Hydrogen Program Organization

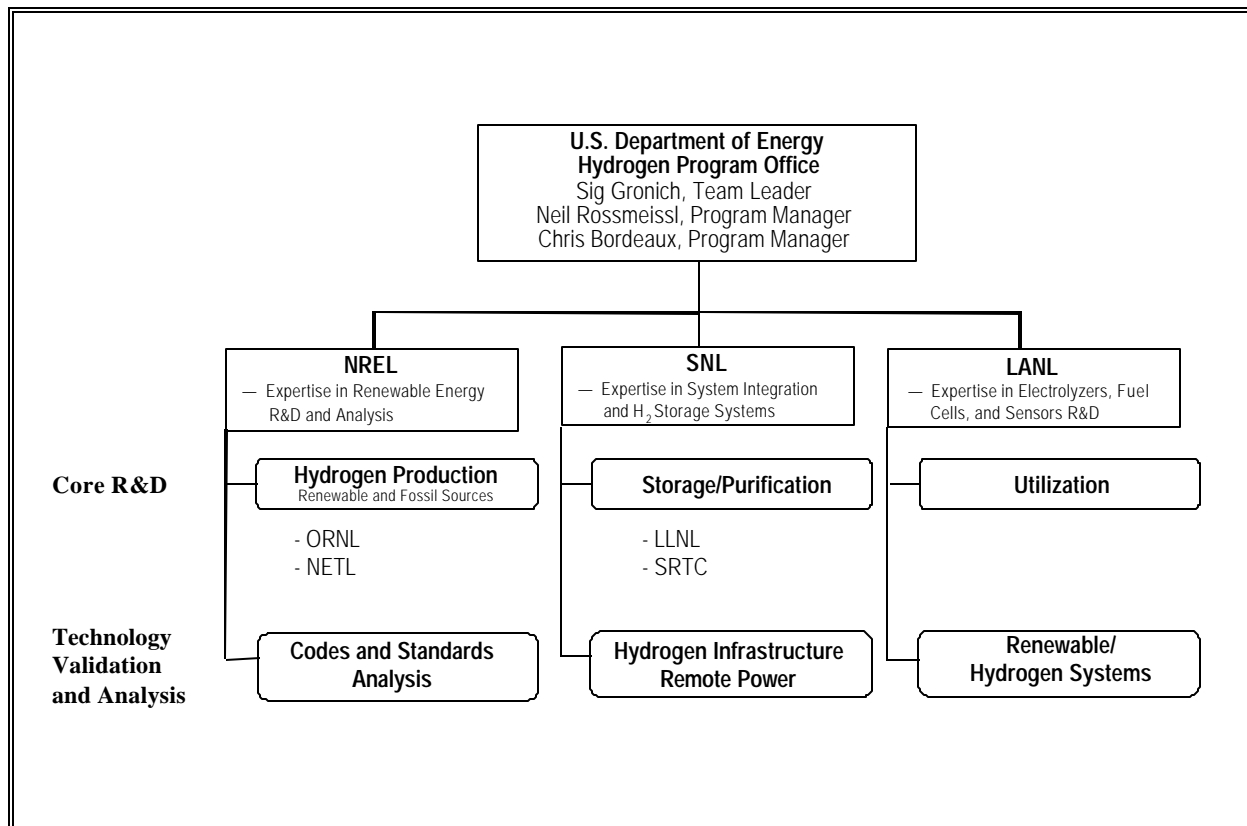
The Hydrogen Program incorporates technical and management assistance provided by key program participants to guide the Program's management and direction, which is established by a DOE Headquarters Management Team. The Hydrogen Technical Advisory Panel (HTAP), NHA, NREL, SNL, LANL, and other Program participants submit input to the Program through both formal and informal mechanisms. These groups provide DOE with recommendations on the implementation and conduct of the Program, multi-year planning and resource allocation between technical and analytical issues. Additionally, independent technical review teams provide DOE with insights on the progress and direction of research and development, and a means by which researchers and industry can exchange information. Technology Road Maps, outlining the path over the next five years toward meeting these objectives, has been used as program guidance. DOE now intends to produce Technology Road Maps that outline the path over the next ten years.

The development of broad-based hydrogen energy systems necessitates interaction and cooperation among a number of crosscutting research and development projects and technologies within the Department and other Federal agencies. The Hydrogen Program is charged with the responsibility (via the Matsunaga and Hydrogen Future Act) to provide this Federal coordination role. DOE has entered into several collaborations in R&D and technology validation with the DOE Offices of Transportation Technologies, Building Technologies, Fossil Energy, and Science as well as the Defense Advanced Research Programs Agency, Defense Conversions Program, Department of Transportation (DOT) and the National Aeronautics and Space Administration (NASA).

The program goals and objectives are met by funding projects within universities, National Laboratories, and industry; monitoring the performance of projects: conducting an Annual Peer Review of all projects; reviewing all technical and programmatic plans with HTAP; circulating monthly program status reports to all of the program principal investigators (PIs) to facilitate communication; and disseminating hydrogen information through publications, participation in technical meetings, and substantive contacts with stakeholders. The activities funded by the Program are classified into three focused areas: a) Core R&D,

b) Technology Validation, and c) Analysis and Technology Transfer. As a result of increased Program funding, many activities that have proven successful R&D phases, are now moving into the technology validation area.

Figure 2.1
DOE Hydrogen Program Organization



3.0 PROGRAM ELEMENTS

Each of the projects described below is accompanied by a milestone (Gantt) chart. Critical milestones are represented by stars in the charts.

3.1 R&D on Hydrogen Production, Storage and Utilization

The objective for this area is to develop critical cost-effective technologies by conducting research and development in the areas of production, storage, transport, and utilization. The work is conducted at universities, national labs, and industry as shown in the table accompanying each section.

3.1.1 Hydrogen Production Research Projects

The FY 2001 hydrogen production projects, summarized in Table 3.1 and 3.2, are broken up into four categories. These include fossil-based and biomass-based production, and electrolytic and photobiological processes. Separation techniques are included in “fossil-based production”, and photoelectrochemical processes are included in the “electrolytic category”.

Table 3.1 Fossil/Biomass Based Production		
Goal: Improve the efficiency and lower the cost of fossil-based and biomass-based hydrogen production processes to \$6-\$8/MMBtu		
Category	Project	Researchers
<i>Fossil-Based Production</i>	Hydrogen Manufacturing Using Plasma Reformers	Mass. Institute of Technology
	Low Cost Hydrogen Production Platform	Praxair, Inc.
	Thermal Dissociation of Methane Using a Solar-Coupled Aerosol Flow Reactor	National Renewable Energy Laboratory (NREL)
	Production of H ₂ by Superadiabatic Decomposition of Hydrogen Sulfide	Gas Technology Institute
	Thermocatalytic CO ₂ – Free Production of Hydrogen from Hydrocarbon Fuels	Florida Solar Energy Center
	Novel Catalytic Fuel Reforming	InnovaTek, Inc.
	Engineering Development of Ceramic Membrane Reactor Systems for converting Natural Gas to Hydrogen and Synthesis Gas for Liquid Transportation Fuels	Air Products and Chemicals, Inc.
	Integrated Ceramic Membrane System for H ₂ Production	Praxair, Inc.
	Production of Hydrobromic Acid from Bromine and Methane for Hydrogen Production	SRT Group
<i>Biomass-Based Production</i>	Biomass to Hydrogen via Fast Pyrolysis and Catalytic Steam Reforming	NREL
	Biomass Pyrolysis for Hydrogen Production	Jet Propulsion Laboratory
	Hydrogen from Biomass for use in Urban Transportation	Clark Atlantic University
	Supercritical Water Partial Oxidation	General Atomics
	Biohydrogen Production from Renewable Organic Wastes	Iowa State University
	Bio-production of Hydrogen Using Thermophilic Bacteria	NETL
	Biological H ₂ from Fuel Gases and from Water	NREL
	Bioreactor Development for Biological H ₂ Production	NREL
<i>Separation & Purification</i>	Separation Membrane Development	SRTC
	Defect-free Thin Film Membrane for H ₂ Separation & Isolation	Sandia National Laboratories

FOSSIL BASED PRODUCTION

Hydrogen Manufacturing Using Plasma Reformers – Massachusetts Institute of Technology

Manufacturing of hydrogen from natural gas, biofuels and other hydrocarbons, is needed for a variety of applications. Plasma technology could provide important improvements in reforming hydrocarbon fuels for the production of hydrogen-rich gas and facilitates use in a wide range of applications. The plasma conditions (high temperatures and a high degree of ionization) can be used to accelerate thermodynamically favorable chemical reactions without a catalyst or provide the energy required for endothermic reforming processes. Plasma reformers can provide a number of advantages:

- Economic operation in small to medium size units
- Operation with a broad range of fuels, including natural gas, diesel and biofuels
- Rapid startup
- Decreased problems of catalyst sensitivity and deterioration
- Compactness and low weight (due to high power density)
- Minimal cost (simple electrodes and power supplies)
- High conversion efficiencies

Hydrogen-rich gas could be efficiently produced in compact plasma reformers with a variety of hydrocarbon fuels including natural gas, biomass, and others. The technology could be used to manufacture hydrogen for a variety of stationary applications including distributed, low pollution electricity generation from fuel cells, turbines and internal combustion engines; hydrogen-refueling gas stations for fuel cell driven cars; and decentralized hydrogen generation for industrial processes. It could also be used for mobile applications (e.g., on-board generation of hydrogen for fuel cell powered vehicles).

Two types of plasma reformers are being investigated. One is a plasmatron using a DC-arc plasma. The other is a low power nonthermal plasma device which MIT has recently developed. Use of this device makes it possible to greatly reduce the specific electrical energy consumption. This reduction more than compensates for the increased energy loss due to increased exothermic energy release of the reforming process.

Task 1: Develop Low Power Plasmatron for Alaska Fuel Cell Project and for Testing at SNL

MIT is estimating that the specific electrical energy consumption with methane will be less than 3 MJ/kg H₂. Operation of low power plasmatron reformer with diesel fuel (for the Alaskan fuel-cell project) will be investigated. The plasmatron will be tested in collaboration with Sandia National Laboratory. SNL needs to upgrade their facility to handle the reformat throughputs from the plasma reformer

Task 2: Increased Hydrogen Production Rates

For higher hydrogen production rates operation (for refueling stations, Fischer-Tropsch plants), a DC arc plasmatron may be superior to a low power plasmatron. Experiments with the DC arc plasmatron will continue in order to determine the regimes where the DC arc plasmatron may be superior to the low power plasmatron. On the other end of the spectrum, MIT proposes to use the low power plasmatron to

investigate hydrogen production rates for use in very low power applications (as low as 1000 W of hydrogen, which is lower than that for the Alaska project), as Auxiliary Power Units.

Task 3: Improved Reactor

The low power plasmatron configuration needs to be integrated into a system with a reaction extension region (a reactor downstream from the plasma and the fuel injection point), a heat exchanger, and various catalytic regions (steam reforming, and high and low temperature water-shifting). Sulfur poisoning of the catalyst will be determined.

Task 4: Pilot Plant

A pilot plant for the generation of hydrogen at an appropriate throughput will be designed. Issues of lifetime and reliability will be addressed. A smaller unit with the low power plasmatron will be designed and constructed.

Hydrogen Manufacturing Using Plasma Reformers Massachusetts Institute of Technology						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Development and Testing of Low Power Plasmatron						
Diesel fuel system integration		◆				
Testing in Sandia National Laboratory			◆			
		◆				
Increased Range of Operation						
Investigate high H ₂ throughput with DC arc		★				
Investigate low H ₂ throughput with low power plasmatron				◆		
Improved Reactor						
System design		◆				
Fuel injection optimization			◆			
Air injection optimization				◆		
Thermal shielding				◆		
Pilot Plant						
Design of plant based on conventional plasmatron			◆			
Polot plant with low power plasma reformer				◆		
FY 2001 Begins October 1, 2000						

Low Cost Hydrogen Production Platform – Praxair, Inc.**Task 1: Concept Definition and Feasibility Analysis**

Define the DFMA-based SMR system in sufficient detail to assess the viability of a business based on selling units to the transportation sector and selling hydrogen to industrial users

Task 2: Phase 2 Detailed Plan and Proposal

Develop a detailed plan and proposal for Phase 2 of the development program. The plan will include a definition of the work to be performed, a definition of accountabilities, a schedule and costs.

Task 3: Phase 3 Preliminary Plan

Develop an outline of the activities to be performed in Phase 3 and prepare a preliminary cost estimate.

Task 4: Project Status Report

Prepare a program status report that documents the essential elements and results of the work performed in Phase 1. This report shall include an overview of the Phase 2 and Phase 3 Plans.

Task 5: Program Management

Perform the management tasks needed to ensure that the work performed under this contract with within budget and schedules. Provide the interface (results, cost, schedule, billings) with DOE Project Management.

A Gantt chart and critical milestone are to be determined.

Thermal Dissociation of Methane Using a Solar-Coupled Aerosol Flow Reactor- National Renewable Energy Laboratory

The basis of this concept is the high temperature thermal dissociation of methane in a solar heated aerosol flow reactor. Methane is dissociated to carbon black and hydrogen in the following reaction:



This reaction was first experimentally demonstrated in 1978, was shown to be fast, and could be carried to 100% completion at temperatures greater than 1815°C. The reactor consisted of an electrically heated aerosol reaction chamber. A small amount of carbon black was introduced to serve as a radiation-absorbing target to initiate the pyrolytic reaction. Once started, the carbon produced continued to serve as the radiation absorbing target and no further addition of carbon was required. Due to the high temperatures involved and the difficulty in heating a gas to those temperatures (by convection from reactor walls), the carbon particles are the key to this process. Although the technical feasibility was conclusively demonstrated, the use of electricity to provide the high temperatures required doomed it economically.

Highly concentrated sunlight can be used to generate the high temperatures needed and provides an environmentally clean option for the production of hydrogen. This process results in 10% increase in the heating value over methane. The solid carbon black can be sold for increased economic value (over the sale of hydrogen) or can be more easily stored or sequestered than can carbon dioxide.

The goal of this work is to demonstrate the technical feasibility of this reaction using highly concentrated sunlight as the energy source and to identify and resolve the specific technical issues needed to move the concept forward. As this process moves through the development path, an industrial partner(s) will be engaged to offer technical guidance to the research, marketing and commercialization experience and cost-sharing of the larger-scale development aspects.

Preliminary economic analyses conducted in FY00 indicated the importance of good reactor performance. The target for reactor efficiency (total enthalpy required/incident solar energy on the receiver) to achieve acceptable economics is 50%. Thus establishing realistic and then improving reactor performance must be a major goal of the technical work. The heat recovery system (an important interface between the solar and conventional portion of the plant) was an area of uncertainty in the initial economic analysis. Here it will be important to design this system for good heat transfer while mitigating the potential effects of carbon fouling.

Work planned for FY01 includes the design and fabrication of a new reactor system for testing at the HFSF; improved definition of process unit operations with emphasis on solar/conventional plant sizing, design and layout; and improved economic analysis with more detailed component models.

Additionally, the work will be documented and presented in appropriate programmatic meetings and to prospective industrial partners.

Task 1: Design, Construction, and Experimental Evaluation of an Optimized Laboratory Reactor

Subtask 1-1: Identify, analyze and evaluate various reactor design concepts. This includes developing methods for effectively dispersing and flowing radiation absorbing particles through the reaction tube, fluid-wall reactor considerations for preventing wall fouling, designing for optimized solar-thermal coupling (location and area for radiative heating), and design and construction of a secondary concentrator for maximized effective energy input.

Subtask 1-2: Improve measurement and analytical methods. Involving upgrading gas flow control system, taking temperature measurement of particles/gases in the reactor, and developing in-line GC/MS gas phase analysis

Task 2: Unit Plant Operations

Subtask 2-1: Solar hardware. This includes designing reactor for pilot scale and its integration of reactor with conventional unit operations and developing the solar plant design concept and field layout.

Subtask 2-2: Conventional hardware. This design will be based on existing carbon black plants, heat recovery options.

Subtask 2-3: Economic evaluation. Improved reactor performance algorithm, incorporating new/modified component models, coordinating the results with the Hydrogen Analysis Team, conducting market studies, determining carbon black market and value, analyzing the hydrogen market, and coupling with solar resource (e.g. siting).

Thermal Dissociation of Methane Using a Solar-Coupled Aerosol Flow Reactor National Renewable Energy Laboratory

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Design, construction, and experimental evaluation of an optimized laboratory reactor						
Select reactor system concept/Complete reactor fabrication			◆			
Complete initial reactor experiments				◆		
Unit plant operations						
Complete pilot plant design concept and component configuration				◆		
Complete economic analysis of pilot plant					★	

FY 2001 Begins October 1, 2000

Production of H₂ by Superadiabatic Decomposition of Hydrogen Sulfide - Gas Technology Institute (GTI)

The goal of this project is to develop a novel process for the production of low cost hydrogen and sulfur by enhanced thermal decomposition of hydrogen sulfide, with no carbon dioxide emissions.

The proposed process uses superadiabatic combustion (SAC) to thermally decompose H₂S to hydrogen and sulfur. A portion of the H₂S is combusted to provide the energy required for decomposition. SAC is based on combustion in the presence of a porous medium with intense heat exchange. As a result, the flame temperature in SAC can significantly exceed the adiabatic flame temperature for the mixture.

The objective for phase 2 of the project is to develop the necessary experimental data to demonstrate the technical and economical viability of the process and to finalize industrial partners for market evaluation and commercial demonstration.

Task 1: Construction of Lab-Scale Unit

A lab-scale SAC-Based H₂S decomposition reactor system will be constructed to obtain the necessary experimental data to verify the technical feasibility of the process. The reactor consists of fixed-beds packed with alumina pellets where hydrogen sulfide is thermally decomposed to hydrogen and sulfur. In this unit H₂S-rich waste gas is mixed with air and fed to the SAC reactor. Off-gas leaving the SAC reactor is cooled to condense sulfur vapors and liquid sulfur is drained and collected. Cooled off-gas is fed to a H₂S separator where unconverted H₂S is removed from the gas stream and recycled to the SAC Reactor. Off-gas leaving the H₂S separator is then fed to a H₂ separator where hydrogen is recovered and the off-gas is discharged to the atmosphere.

Task 2: Parametric Studies

In this task, based on the test plan developed in Phase 1, a number of tests will be conducted in the lab-scale SAC reactor unit to determine the effects of operating parameters on the performance of the process. The parameters to be studied in these tests will include inlet fuel gas composition, equivalence ratio, gas residence time, temperature, and the porous media material.

Task 3: Technical and Economic Feasibility Verification

The data generated in Task 2 will be thoroughly analyzed to verify the technical feasibility of the process. Based on these results, the computer model used in Phase 1 for predicting SAC performance will be updated. The process design for SAC will be updated and optimized to maximize system efficiency and hydrogen production. The system cost will be updated based on the optimized process design.

Task 4: Update Market and Economic Study

The results obtained in Task 3 will be used to validate the market and economic viability of the process. Evaluation of potential markets will include analysis of both the sulfur recovery markets as well as hydrogen and sulfur end-user markets. Factors considered in the analysis will include:

- Current and projected hydrogen and sulfur prices
- Status of competing hydrogen production and combined hydrogen and sulfur recovery processes under development
- Current size and demand projections for the various hydrogen market sectors, including petroleum refining, ammonia, methanol, and fuels

- Current size and demand projections for sulfur market sectors, including sulfuric acid, fertilizers, etc.
- Information on the sulfur recovery, hydrogen and sulfur markets will be used to determine the most favorable potential settings for deployment of the SAC hydrogen production technology.

**Production of H₂ By Superadiabatic Decomposition of Hydrogen Sulfide
Gas Technology Institute (GTI)**

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Construction of Lab-scale Unit						
Complete construction of the unit			◆			
Complete unit shakedown				◆		
Parametric Studies						
Complete parametric studies						◆
Technical and Economic Feasibility Verification						
Complete verification of technical feasibility						★

FY 2001 Begins October 1, 2000

Thermocatalytic CO₂-free Production of Hydrogen from Hydrocarbon Fuels – Florida Solar Energy Center (FSEC)

Conventional processes of hydrogen production are among the major producers of CO₂ emissions. Perspectives of CO₂ sequestration are actively discussed in the literature, however, it is an energy intensive and costly process associated with uncertain ecological consequences. The main objective of this work is to develop a novel process for CO₂-free production of hydrogen and carbon from hydrocarbon fuels as a viable alternative to the conventional processes (e.g. steam reforming) coupled with CO₂ sequestration. The technical approach is based on a single-step decomposition (or pyrolysis) of hydrocarbons over carbon catalysts in an air/water free environment. This approach eliminates the need for water-gas shift, CO₂ removal and catalyst regeneration stages, which significantly simplifies the process.

The project strives to accomplish the following technical goals: a) establish the basic scientific and engineering data necessary for the development of a process development unit (PDU) and, ultimately, a commercial unit, b) design, fabricate and test a multi-fuel thermocatalytic reactor (TCR) for CO/CO₂-free production of hydrogen-rich gas and carbon, and c) test the performance of the TCR in combination with a PEM fuel cell. To meet these goals, FSEC will collaborate with the following industrial partners: Universal Oil Products (UOP), Energy Partners, Inc. and Air Liquide Medal, L.P.

Task 1: Optimization of Hydrocarbon Pyrolysis Reaction

Conduct reaction optimization studies to increase overall hydrogen yield by optimization of the operational parameters (e.g. temperature, residence time) and catalyst surface area, and carbon crystallite size. The long term stability of the selected carbon catalysts will be improved by involving an in-situ generation of catalytically active carbon species. The factors that may influence the deactivation of carbon catalysts will be studied. This task will also determine the effects of hydrocarbons of different classes, including saturated, unsaturated and aromatic hydrocarbons, on the activity and long term stability of selected carbon catalysts.

Task 2: Process Engineering Development

Conduct system engineering studies by evaluating heat and mass transfer within the thermocatalytic reactor. A moving bed catalytic reactor will be engineered to test the feasibility of simultaneous production of hydrogen and removal of carbon from the reactor. Methane, propane and gasoline will be used as feedstocks. This task will also include development of a detailed process flow sheet with material and energy balances using methane and other feedstocks. These flow sheets will be used for techno-economic analysis of the different process options. A miniature hydrocarbon fuel reformer for portable applications focusing on evaluation of different reactor designs targeted for small-scale hydrogen production units will also be developed.

Task 3: Demonstrate 1 kW Hydrogen Production Unit and Evaluate its Performance

Design, construct and test a 1 kW multi-fuel thermocatalytic reactor for producing hydrogen-rich gas and carbon, and evaluate its performance. Methane, propane and gasoline will be used as feedstocks for the reactor. Develop laboratory scale data for more detailed process design and techno-economic analysis. FSEC will also collaborate with their industrial partner to test the performance of the TCR in combination with a PEM fuel cell. A techno-economic and system analysis of the process will be performed,

including a sensitivity analysis based on the expected range of feedstock cost, hydrogen yield and byproduct carbon cost and an assessment of the market potential for carbon produced.

Thermocatalytic CO ₂ -free Production of Hydrogen from Hydrocarbon Fuels Florida Solar Energy Center						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Optimization of Hydrocarbon Pyrolysis Reaction						
Conduct reaction optimization studies			◆			
Complete evaluation of long term stability of carbon catalysts				◆		
Complete studies on the effect of different hydrocarbons		◆				
Process Engineering Development						
Conduct evaluation of heat and mass transfer in the system				◆		
Develop detailed process flow sheet					◆	
Complete development of a miniature hydrocarbon reformer				◆		
Demonstrate 1 kW Hydrogen Production Unit						
Demonstrate 1 kW multi-fuel thermocatalytic reactor				★		
Test the reactor in combination with PEM fuel cell					◆	
Conduct techno-economic and system analysis						◆
FY 2001 Begins October 1, 2000						

Novel Catalytic Fuel Reforming – InnovaTek, Inc..

The ultimate goal of this project is to develop a multi-fueled reformer for the production of clean hydrogen. Advanced separation technology will be incorporated to provide a pure output stream of hydrogen to be used as a fuel stream for a compatibly sized PEM fuel cell for electrical generation.

InnovaTek is applying the advantages of microtechnology in the development of catalytic fuel reforming. The specific problem being addressed here is an energy conversion process to provide clean hydrogen from diesel and natural gas. This approach to fuel processing provides a revolutionary breakthrough in terms of system size, weight, and dynamic response when compared to more conventional processing carried out in standard packed bed reactors.

Although the program and tasks this year are primarily focused on diesel fuel (or JP-8), much of the program includes testing with methane, dodecane and other simplified surrogates for diesel fuel. When operability with diesel fuel is demonstrated, only minor changes will be required for operation with any other fuel system. Because of its methane content, natural gas will require the most significant changes to the system. Although an elaborate system of fuel atomization will probably not be required, the system designed for diesel will be used in the natural gas system modification. The injector/atomizer system will continue to provide necessary mixing of the natural gas into the steam reformer. The most significant change required will be in the operating temperature of the reformer.

Task 1: Diesel Fuel Injector Development

The purpose of this study is to design and test an injector (i.e., atomization and mixing) system specifically engineered for the high temperature reforming of diesel fuel in a catalytic micro channel reactor. The end result of this work will be the design and delivery of a functioning, compatible atomizer-mixer injector for integration into the InnovaTek diesel fuel reformer design.

Task 2: Hydrogen Separation Technology

The purpose of this task is to develop a membrane separation system for supplying a pure hydrogen product stream. This system will remove other products, CO, CO₂, hydrocarbon fragments and sulfur, from the diesel reformer process stream. The reject stream from the membrane will be recycled to the system burner to generate operating heat. Appropriately sized membrane tubes will be fabricated into a manifold design with a capability to deliver hydrogen at a rate of 1.2 LPM for the first lab demonstration and then 12 LPM for the full-scale work. The final unit will become part of an integrated reformer unit for testing and confirmation.

Task 3: Reject Stream Recycle

Recycling of the reject stream from the membrane separator will be studied for two possible alternatives uses. Depending on the composition of the stream one possible use is for it to be used as fuel in the burner that provides system heat. The other use, if water and CO are high and other hydrocarbon fragments low, will be to subject the stream to a second stage of low temperature water gas shift followed by membrane separation. The decision reached in the modeling trade study will establish the direction of further development with regard to how the membrane reject stream is processed. If secondary waste gas stream processing is deemed the route of choice, then the issue of autothermal reforming also becomes a possibility.

Task 4: Heat Exchange and Utilization

The key to efficient operation of the reformer will be the capability to utilize heat efficiently. The HYSYS program modeling for the step-wise reaction breakdown will be used as a basis for sizing and designing exchange components for dealing efficiently with process heat in the reactor.

Task 5: System Sensors and Controls

System sensor and control work will begin during later phases of this work. Ultimately, sensors will be required to monitor and control all aspects of the reformer operation. These specifically include start-up, normal operation and shutdown. In addition, operational safety concerns will be addressed in the design of the sensor/control system. At this stage of work, the final laboratory prototype reformer will be equipped with laboratory scale sensor and controller devices.

Task 6: Peripheral Hardware

Consideration of peripheral hardware will include selection of delivery pumps for diesel and water feed streams. Candidate units will need to provide uniform feed rate control at pressures from 50 to 100 psi and be compatible with the chemistry of the feed streams. Small size and ruggedness will also be considered as critical selection criteria.

Task 7: System Integration and Testing

Reactor components resulting from the design and fabrication work listed above will be integrated into a laboratory operating prototype reactor. Additional components will include the burner unit and the catalytic plasma reformer. System integration work will be accomplished in cooperation with work being done on the U.S. Army Diesel Reformer Project.

Task 8: System Tests with Natural Gas Fuel

The diesel system prototype reformer will be used in tests with natural gas as a fuel. In these tests, it is anticipated that operating temperature will need to be increased by about 150°C over that used in the diesel reforming tests.

Task 9: Plan for Development of a Stationary Natural Gas Reformer

Following an analysis of natural gas testing, a plan for developing a stationary natural gas reformer will be developed.

Task 10: Design for Manufacturing

Because cost is such a critical issue associated with the commercial viability of fuel cells, it is imperative to design the fuel processing technology for economical production. InnovaTek will employ the following factors to guide the design tasks and will further analyze components to improve effectiveness of design to improve manufacturability:

- Simplicity—reduce number and complexity of parts
- Standard materials and components
- Design appropriate to expected level of performance
- Use materials that are easily processed

- Avoid secondary operations
- Utilize special process characteristics, e.g., computer-controlled equipment

Novel Catalytic Fuel Reforming InnovaTek, Inc.						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Diesel Fuel Injector Development		◆				
Hydrogen Separation Technology		◆				
Reject Stream Recycle			◆			
Heat Exchange and Utilization				◆		
System Sensors and Controls					◆	
Peripheral Hardware					◆	
System Integration and Testing						◆
Operating Prototype Reactor						★
System Tests with Natural Gas Fuel						◆
FY 2001 Begins October 1, 2000						

Engineering Development of Ceramic Membrane Reactor Systems for Converting Natural Gas to Hydrogen and Synthesis Gas for Liquid Transportation Fuels – Air Products and Chemicals, Inc.

The objective of this program is to research, develop and demonstrate a novel ceramic membrane reactor system utilizing a ion transport membrane (ITM) for the low-cost conversion of natural gas to hydrogen and synthesis gas for liquid transportation fuels: the ITM H2 and ITM Syngas processes. Through an eight-year, three-phase program, the technology will be developed and scaled up to obtain the technical, engineering, operating and economic data necessary for the final step to full commercialization of hydrogen generation and syngas for gas-to-liquid (GTL) processes.

Phase 2 of the program, Engineering and Development of an ITM Syngas / ITM H2 PDU and SEP, was initiated in FY2000. Phase 2, which extends for 3.5 years, will validate process concepts in two stages of scaleup and create an engineering, operating and economic database. The following tasks will be completed in Phase 2.

Task 1: Commercial Plant Economic Evaluation

Air Products, Chevron, McDermott and Norsk Hydro will develop advanced ITM H2 and ITM Syngas processes, with input from the University of Alaska. The economics of operation at the commercial-plant scale will be evaluated based on the results of the Phase 2 program.

Task 2: Materials and Seals Development and Evaluation

Air Products, Eltron Research and Penn State University will obtain laboratory-scale statistical performance and lifetime data under ITM H2 and ITM Syngas process conditions. Ceramtec will fabricate the ITM membrane / seal samples for testing, with input from Norsk Hydro, Pacific Northwest National Laboratory and the University of Pennsylvania.

Task 3: ITM Syngas Membrane and Module Design and Fabrication

Air Products, Ceramtec and McDermott will design membrane reactors for the ITM H2 / ITM Syngas processes at the Process Development Unit (PDU), Sub-scale Engineering Prototype (SEP) and commercial scales. Ceramtec will fabricate sub-scale membrane modules for testing in the PDU. Ceramtec will also scale up the fabrication of the membrane reactor modules in a Production Development Facility (PDF) to supply the requirements of the SEP.

Task 4: Nominal 24 MSCFD ITM Syngas PDU

Air Products will demonstrate the components of the ITM H2 / ITM Syngas technology in a laboratory PDU. The PDU will operate at an equivalent of 24 MSCFD of syngas capacity, and will performance test sub-scale planar membranes under commercial process operating conditions.

Task 5: Nominal 500 MSCFD ITM Syngas SEP

A SEP unit will be constructed and used to demonstrate the ITM H2 and ITM Syngas technology at up to an equivalent of 500 MSCFD of syngas capacity.

At the end of Phase 2, the projected commercial-plant economics for ITM H₂ and ITM Syngas will be re-evaluated by Air Products, Chevron, McDermott and Norsk Hydro, based on the results from the PDU and SEP operations. Three commercial-scale applications will be evaluated: hydrogen generation, offshore GTL, and remote Alaskan North Slope GTL.

**Engineering Development of Ceramic Membrane Reactor Systems for Converting Natural Gas to Hydrogen
and Synthesis Gas for Liquid Transportation Fuels
Air Products and Chemicals, Inc.**

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Evaluate Advanced Processes						
Define advanced ITM H ₂ /ITM Syngas processes			◆			
Evaluate ITM Materials and Seals						
Test sub-scale planar membranes at high pressure		◆				
Test tubular membranes and seals at high pressure				◆		
ITM Syngas Membrane & Modular Fabrication						
Select PDU module design	◆					
Fabricate sub-scale PDU modules			◆			
Design SEP membrane and start fabrication						◆
Nominal 24 MSCFD ITM Syngas/ITM H₂ PDU						
Conduct techno-economic and system analysis				◆		
Performance test on subscale modules in PDU					★	
Nominal 500 MSCFD ITM Syngas/ITM H₂ SEP						
Define SEP scope					◆	

FY 2001 Begins October 1, 2000

Integrated Ceramic Membrane System for Hydrogen Production – Praxair, Inc.

Information not available at time of printing

Production of Hydrobromic Acid From Bromine and Methane for Hydrogen Production – SRT Group, Inc.

SRT will work together with Sandia National Laboratories and the Wyoming Research Institute to producing a prototype system based on the reaction between bromine and methane for the production of hydrobromic acid and the electrolysis of the acid back to hydrogen and bromine for a complete cycle. After a pre-commercial prototype reactor system is developed, the electrolyzer shall be replaced with a reversible fuel cell to enable energy storage.

The SRT process entails the reaction of bromine with methane to produce hydrogen bromide and carbon. The hydrogen bromide produced can be reacted with water to produce hydrobromic acid that can be stored in a fiberglass tank or maintained as hydrogen bromide gas in a high-pressure stainless steel tank. Both chemicals can be electrolyzed for the production of $H_{2(g)}$ and recovery of $Br_{2(l)}$. In this manner, hydrogen is generated without greenhouse gas emissions. SRT proposes to conduct the research to develop a bromine reformer that reacts bromine liquid and natural gas in an exothermic reaction to produce hydrobromic acid. This reformer will be integrated with a 9 kW non-regenerative electrolyzer in a system using hydrobromic acid to allow for testing and modeling of the electrolyzer. Subsystem testing and development of the bromine tank, control system and ancillary systems are included. Included in this research effort is the investigation of the two storage concepts, as hydrogen bromide and hydrobromic acid. These two approaches will be analyzed for capital cost, safety, and process flexibility.

Task 1: Materials Development

Materials that are used in the reactor must have good thermal stability, have mechanical properties that will allow manufacture of seals, threads or assembly points and be chemically stable to minimize corrosion. Researchers in this task will investigate a series of materials that have properties that can be commercially fabricated into future reactors. In a parallel effort, the reactor will be designed to provide flexibility for the experimental program. Parameters which will be studied include methods for varying the residence time of the reaction, injection pressure and temperature of the natural gas and bromine, swirl pattern, recirculation of the effluent, and heat transfer rate to vary the temperature profile of the reactor without secondary heating or cooling

Task 2: Bench Scale Experiments

The laboratory apparatus is intended to provide data that can be used to develop a chemical kinetics equation, rather than demonstrate the process as it might be used in production. An experimental reactor will be used that will allow a broad envelope of reaction conditions to be evaluated. The most important variables that define this envelope are the reactor temperature, the ratios of the reactants in the feedstock, and, the residence time in the reactor (flow rate).

Task 3: Computer Modeling

Calculations of both equilibrium chemical behavior and reaction kinetics are required to interpret the experimental data collected. These calculations will be performed using the CHEMKIN computer program and its associated thermodynamic and kinetic databases.

Additional information may need to be input to complete the database for computations. The results of the laboratory experiments will be compared with the predictions of the computations to refine the reaction rate equations. The equilibrium calculations will enable the next generation experimental

apparatus to be designed with full regard for all of the reaction products that may be formed. Such calculations also provide useful information regarding the energetics of the reactions that are useful for engineering design.

Task 4: Reactor Scale-up

The purpose of this task is to scale-up the process toward a working prototype. The work consists of several tasks, collecting and evaluating all available information, including data from previous work, define a test matrix to refine the data needed for to generate required data set for process scale-up, analyze and confirm scale-up data, materials, and component compatibility issues, devise control schemes for process start-up, shut down, and process control, address reactant containment, reactant and product storage issues, and effluent purification, and validate all the results prior to building any hardware.

Task 5: Analytical Methods

A significant effort was expended by SRT to improve the analytical techniques for quantifying the compounds in the effluent stream. The mass of the samples in the collection tubes were measured. The aqueous solution density was determined. A spectrophotometric method using two wavelengths for determining the bromine concentration in aqueous solutions containing HBr was developed. The titration of HBr with NaOH was improved by using a derivative of the titration curve. Non-condensable gases were analyzed with a gas chromatograph (GC) method. These methods will be evaluated during the early phases of the work. Alternative methods may be developed to improve the closure of the mass and energy balances.

Task 6: Economic Analysis

Improve the economic analysis during the scale-up experiments. With an improved energy and mass balance, those terms needed for the calculation of the system efficiency will be more accurate.

Production of Hydrobromic Acid from Bromine and Methane for Hydrogen Production SRT Group, Inc.

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Review Prior Data and Related	◆					
Bench Scale Experiments						◆
Conceptual Process Flow Sheet and Reactor				◆		
Facilities Preparation		◆				
Components and Hardware					◆	
System Assembly and Start-up						◆
Plant Operations and Process Optimization						◆
SO ₂ Abatement/Hydrogen					◆	
Economic					◆	
Annual					◆	
Project					◆	

FY 2001 Begins October 1, 2000

BIOMASS-BASED PRODUCTION

Biomass to Hydrogen via Fast Pyrolysis and Catalytic Steam Reforming – National Renewable Energy Laboratory

At present, the commercial production of hydrogen is essentially carried out by catalytic steam reforming of hydrocarbons: natural gas and naphtha. These processes generate, as a side product, carbon dioxide in amounts equal to those of combustion operations, thus contributing to the greenhouse effect. Renewable biomass is an attractive alternative to fossil feedstocks for the production of hydrogen because of essentially zero net CO₂ impact. Biomass includes wood and agricultural residues, municipal solid wastes, industrial wastes from biomass processing (such as pulp and paper operations) as well as dedicated herbaceous and short rotation woody crops. These feedstocks could become available regionally via a diversified choice of species and residues characteristic of each region. The challenge is to convert the biomass into hydrogen at a cost similar to that from existing hydrocarbon-based reforming technologies. If successful, this strategy would substantially help the economic development and diversification of rural areas.

The project has the following goals:

- Establish a scientific and technological data base for the conversion of biomass into hydrogen via advanced thermochemical processes (i.e. fast pyrolysis followed by catalytic steam reforming)
- Integrate hydrogen production with key co-products derived from biomass in order to improve the economics
- Implement the process concept at the regional level in an effort towards sustainable development

This project started in December 1993. A dedicated team of researchers has, since then, established scientific proof that biomass pyrolysis oil (i.e. bio-oil) can be steam-reformed to generate hydrogen. The study was initiated using model compounds, which are major components of pyrolysis oils. It demonstrated, first at the micro-reactor level, then in a bench scale unit, that acetic acid, hydroxyacetaldehyde, various alcohols, furfural, and methoxyphenols can be efficiently converted to hydrogen (and carbon oxides) using commercial nickel-based catalysts. Subsequent technoeconomic evaluation had shown that the strategy coupling biomass pyrolysis with steam reforming could be commercially attractive if specific components or fractions of pyrolysis oils were marketed as co-products for different applications. The first case considered has been the isolation of the lignin-derived fraction present in the pyrolysis oil. Such fraction, after a post-treatment, becomes a co-product that can replace phenol in adhesives formulation. The remaining, carbohydrate-derived, fraction of the pyrolysis oils can then be used for the production of hydrogen that could be generated at competitive costs with current market prices. NRELs experiments, carried out in the fixed-bed reactor, have shown that in initial stages of the process the carbohydrate-derived fraction of poplar pyrolysis oil could be almost stoichiometrically converted to hydrogen. However, the process performance decreased with time because of char and coke deposition on the catalyst surface and in the bed itself limiting the reforming cycle to two or three hours. This cycle was even shorter when whole bio-oil or polymeric biomass-derived liquids (hemicellulose-rich fraction from biomass steam fractionation process) were used as feedstocks for hydrogen production. In order to improve the process performance NREL decided to use a fluidized bed reactor instead of the fixed-bed for the reforming the whole bio-oil and its fractions. The fluidized bed configuration provides better contact between the reactants and the catalyst. The latter has thus an extended time-on-stream. The reforming experiments carried out to date in the fluidized bed system with the carbohydrate-derived fraction of pyrolysis oils have shown promising results. The catalyst shows a slow decrease in activity with time, which NREL has proven can be overcome by catalyst regeneration, either on- or off-stream. The mechanical strength of the catalyst is the last issue that remains to be resolved. Commercial reforming

catalysts are currently designed and used for fixed-bed applications. The particles obtained by grounding the available pelletized commercial catalysts tend to disaggregate during the fluidization process. NREL needs to find an adequate method to strengthen the catalyst mechanically for use in the fluid bed system. At present, NREL feels confident that the process can be taken to the next stage of development: scale up and integration of the fluid bed catalytic reformer with a pyrolysis reactor operating at a capacity of 10 kg/h of biomass.

Task 1: Catalyst Development

NREL's previous experiments showed that a catalyst formulation, C11-NK manufactured by Süd-Chemie (formerly United Catalysts), could efficiently operate without regeneration for almost 100 hours. NREL will determine the optimum duration of the reforming and regeneration cycles and will establish the efficiency of the regenerated catalyst as a function of time-on-stream and number of regeneration cycles. Tests will be carried out using the existing fluidized bed reactor system. The catalyst activity will be measured as the efficiency of conversion of biomass liquids to hydrogen. Regeneration will be performed using steam and carbon dioxide, the latter being the major process co-product. The emphasis will be also put on the evaluation of the catalyst losses due to mechanical attrition.

During previous tests NREL has documented that a significant fraction of the commercial catalyst particles used in the fluidized bed process were entrained from the reactor. Commercial reforming catalysts are currently designed and used for fixed-bed applications. For the fluid bed operation NREL ground the commercial catalyst, obtained in the form of extruded rings, to the particle size desired for the operation. However, the ground particles undergo undesired attrition during the process. In order to solve this problem NREL has initiated a collaboration with Süd-Chemie and BEPEX, a company in Minnesota, on the preparation of a mechanically strong catalyst. In this task, a research fluidizable catalyst from Süd-Chemie will be obtained and tested in NREL's process. Also, a sample will be prepared by BEPEX using their patented method of agglomeration by compaction. NREL expects that the new materials will exhibit improved mechanical properties together with the same high chemical activity found in the C11-NK catalyst. These materials will be characterized for physical and chemical properties. The best material will undergo lifetime tests with selected process conditions.

Task 2: Reactor Development

Steam reforming is an endothermic process that requires substantial amounts of heat. In these experiments, an external electric heating has been used to maintain the process temperature. In a larger scale unit heat will have to be supplied by a cheaper source of energy. A possible option is to use the feedstock (bio-oil or its fractions) for this purpose. Probably the most efficient way to do this is by partially oxidizing the feed in the catalytic bed. This will result in reducing hydrogen yields (by approximately 20%) but will provide energy necessary for reforming. In the past year, NREL has attempted to verify if a combination of reforming with partial oxidation could supply required process energy and prevent formation of carbon deposits on the catalyst (or their immediate removal) during the processing of pyrolysis liquids. So far, the research has shown that the catalyst activity for the reforming reactions rapidly decreases with time probably as a result of the catalyst oxidation (active form is Ni metal). In this task NREL will apply a different strategy: partial oxidation of the feedstock (bio-oil or its fractions) prior to contact with the catalyst. NREL is planning to modify the reactor and use its preheater section for partial oxidation. Hot gases formed in this section will be used to heat the reformer. NREL will apply both natural gas and bio-oil to provide energy necessary for reforming.

NREL's project has reached the stage at which scale up to a 10 kg/h fluid bed reforming unit is going to proceed via the partnership mentioned in other sections of the AOP. The need for a model that would facilitate the scale up as well as operational strategies is being addressed in conjunction with Dr. Josette Bellan at JPL. NREL will support the work of JPL by providing experimental information, particularly on the kinetics, that can facilitate the development of a reaction model based on first principles. Although such a model will be specific to the fluid bed reforming, it may pave the way for additional extensions of the model to other processes in which biomass is converted using fluid bed technology. The codes developed at JPL will be progressively transferred and tested at NREL as predictive tools for the fluid bed operation. Data obtained at NREL will, in turn, be relayed to JPL for the adjustment of the models.

Task 3. Feedstock Research

NREL is planning to explore co-processing natural gas with biomass pyrolysis liquids. Successful production of hydrogen by co-processing biomass-derived materials with natural gas would have similar advantages to co-firing biomass with the fossil fuels. This activity is of interest to the NREL/NETL effort (Memorandum of Understanding – MOU) that is being developed to explore areas of cooperation between the two labs.

Hemicellulose-rich aqueous solutions from biomass fractionation processes and waste glycerin from bio-diesel plants that were studied in the last two years appear to be good candidates for steam reforming processing (Milestone reports, June 1999 and June 2000). NREL intends to carry out the reforming tests on trap grease from food processing that has a high potential for producing hydrogen and can be obtained at a low price throughout the country. Samples of trap grease will be obtained, analyzed, pretreated (if necessary) then steam reformed using the 2"-diameter fluidized bed reactor.

For each feedstock, process conditions will be optimized considering hydrogen yield and catalyst time-on-stream as the base criteria. Material balances and hydrogen yields obtained will be used for preliminary technoeconomic assessment of the technology providing hydrogen production prices from low-cost feeds.

Biomass to Hydrogen via Fast Pyrolysis and Catalytic Steam Reforming National Renewable Energy Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Catalyst Development						
Catalyst Development					★	
Reactor Development						
Demonstrate partial oxidation/reforming reactor operation.				◆		
Feedstock Research						
Demonstrate the feasibility of catalytic steam reforming of selected carbonaceous materials.			◆			
FY 2001 Begins October 1, 2000						

Biomass Pyrolysis for Hydrogen Production – Jet Propulsion Laboratory

This task is performed in conjunction with NREL in the context of hydrogen production from biomass using fluidized bed reactors. Competing processes in fluidized bed reactors making uncertain which of the processes will prevail in a given operation regime, the Jet Propulsion Laboratory (JPL) modeling studies and simulations provide a financially economic way of indicating reactor optimization and scaling. The results obtained during FY00 showed that JPL has currently arrived at the point where the NREL fluidized bed reactor development may benefit from the results obtained with their code. Therefore, it is envisaged that progress will be continued during FY01 in two parallel directions: (1) initiation of practical utilization/development of the current code at NREL described herein in Task 1, and (2) continuing fundamental development of the fluidized bed reactor model at JPL (see Tasks 2 and 3 below).

Task 1: Code Transfer to NREL

To enable the practical utilization/development, the code will be transferred to NREL personnel. This transfer will occur at JPL where designated NREL personnel will come to learn the details of the model and code, and learn to exercise it. It is envisaged that several sessions of multiple days each will be necessary to accomplish the transfer. Additionally, JPL personnel will be available to NREL personnel for elucidation of the code and advice in implementing desired changes at times between the visits. Since the code is built in modular fashion, it is envisaged that these modules will be changed at will by NREL personnel to suit the situation under immediate consideration. Furthermore, additional modules could be added by NREL personnel to the code, as appropriate, to describe practical situations under immediate consideration.

Task 2: Finalization of the Fluidized Bed Reactor, Dual Purpose (Pyrolyzer And Reformer) Model

To mitigate segregation of biomass and sand for the pyrolyzer Jet Propulsion Laboratory proposed feeding biomass into the fluidized bed through the side wall at the bottom, or simply through the bottom of the reactor. In this manner, the interaction time of biomass and sand will be maximized, enhancing pyrolysis. These results are currently being documented for a refereed journal article. It is foreseen that for the reformer (see Task 3 below), segregation will also occur between the catalyzer pellets and the cenospheres (see definition below), and in this case it will be beneficial because it will allow the elutriation of the latter for the purpose of removal from the bed and perhaps for further utilization as combustible fuel to provide the heat necessary for the reformer. These ideas will have to be confirmed by simulations in Task 3.

During FY01, the turbulence model and code will be finalized and a set of simulations will be conducted to validate the model. It has been argued (Balzer et al., EDF Technical Report HE-44/93.13B, 1993) that the precise turbulence model is not very critical in the dense regions of the bed as the particle motion is completely dominated by collisions. However, in the present application the turbulence changes the hydrodynamic time scale, and therefore affects the chemical reactions through the influence that it has on heat transfer. The gas phase turbulence model is also important in the prediction of the recirculating gas flow pattern in and around the 'bubbles' (Balzer et al., 1993) in the fluidized bed which in turn may have effects on the thermal and reactive behavior of the bed.

Candidate experimental data for model validation for the pyrolyzer are (1) Scott, D. S. et al., "The role of temperature in the fast pyrolysis of cellulose and wood", *I&EC Research*, 27, 8-15, 1988, (2) Scott, D. S. and Piskorz, J., "The continuous flash pyrolysis of biomass", *Can. J. Chem. Eng.*, 62, 404-412, 1984, (3) Scott, D. S. and Piskorz, J., "The flash pyrolysis of aspen-poplar wood", *Can. J. Chem. Eng.*, 60, 666-674, 1982, (4) Liden, A. G. et al., "A kinetic model for the production of liquids from the flash pyrolysis of biomass", *Chem. Eng. Comm.*, 65, 207-221, 1988, (5) Stiles, H. N. and Kandiyoti, R. "Secondary reactions of flash pyrolysis tars measured in a fluidized bed pyrolysis reactor with some novel design features", *Fuel*, 68, 275-282, 1989, (6) Piskorz, J., et al.,

“Fast pyrolysis of sweet sorghum and sweet sorghum bagasse”, *J. Analytical and Applied Pyrolysis*, 46, 15-29, 1998, and (7) Scott, D. S. et al., “A second look at fast pyrolysis of biomass – the RTI process”, *J. Analytical and Applied Pyrolysis*, 51, 23-37, 1999.

Once the model will be validated, results will be obtained describing the parametric variation of tar yield with (1) fluidized gas velocity and temperature, (2) biomass particle initial (i.e. feed) temperature and feed rate, (3) feed stock (biomass with different composition in terms of cellulose, hemicellulose and lignin will be tested), (4) particle size, (5) reactor wall temperature and (6) feed location in the reactor. The optimal regime for tar production thus identified will describe a parametric ‘envelope’ which will constitute the target for the NREL reactor optimization. The purpose of this study is to investigate the coupling between the biomass particle residence time and the sand temperature for maximizing tar yield. In particular, Jet Propulsion Laboratory wants to predict the tar yield versus the temperature of the walls and the sand, the tar yield versus time and versus the gas velocity at the distributor.

Furthermore, the model will be exercised for reactor scale-up; both self-similar and non-proportional scales will be explored. This information is crucial for the success of the NREL pyrolyzer, since the tar collected depends upon the rate at which tar is produced competing with the rate at which tar is converted into gas. All these results will be documented in the refereed technical literature.

Task 3: The Fluidized Bed Reformer

During FY01 Jet Propulsion Laboratory will initiate the modeling of the NREL fluidized bed reformer *per se*. In this reformer, tar formed in the fluidized bed pyrolyzer will be injected in the form of a dilute spray at an optimal location to be determined from this study. The optimal location is defined as that which maximizes the hydrogen yield from the reforming reactions. These reforming reactions are catalyzed by solid particles that constitute the fluidized material in the bed. According to their NREL colleagues (and confirmed by the literature), while part of the fluid in the drops evaporates and provides the fuel for the reforming reactions, the remaining part becomes eventually a carbonaceous particle having a central ‘blowhole’; the particle is called a ‘cenosphere’. This type of particle is obtained during the evaporation of all viscous, heavy fuels. Its formation is due to asphaltenes in fuels resulting from the low end of the distillation process; for bio-oils, its production is due to oligomeric lignins present in the tar. The blowhole is the result of microexplosions occurring as the limit of superheat for the more volatile species in the tar is reached inside the drop. These particles not only represent a waste of tar and reduce the hydrogen yield, but also represent a problem in that they have to be removed from the bed. Therefore, the ultimate goals of this JPL study are to recommend:

- spray injection location for maximizing the hydrogen yield for a given set of operating parameters,
- regime of operating parameters that will optimize hydrogen yield, and
- location where the cenospheres could be easily removed. Jet Propulsion Laboratory propose burning these cenospheres to provide part of the heat in the fluidized gas and render the process more energy efficient.

The multiclass fluidized bed model developed in Task 2 above will serve as the major building block for this model. In this task the pyrolyzer model for the binary particle classes will be the catalyst and the cenospheres. The pyrolyzer segregation of particles will be desirable to enable cenosphere removal without removal of the catalyst. The specific submodels that must be added to the fluidized reactor model to enable hydrogen prediction include the spray injection and drop evaporation, criterion for cenosphere formation, and evolution of hydrogen from the reforming reaction in the gas phase and upon contact with the catalyst. The knowledge that must be evaluated to enable the addition of these submodels is as follows:

- The differential fuel evaporation of a bio-oil drop
- The drop/cenosphere mass ratio for a bio-oil drop

- The kinetic parameters and heat of reaction for a 'reduced' (i.e. global) steam reforming reaction of the evaporated species
- Kinetic parameters and heat of reaction for catalytic reforming of the evaporated species

To enable the accurate formulation of these models, a critical literature review will be undertaken. The current information will be evaluated to enable further state-of-the-art modeling.

Basically, it is essential to understand that the challenge of the JPL fluidized bed reactor model is to accurately describe the catalytic steam reforming coupled with fluid-dynamic profiles characteristic of the NREL reformer design where the sprayed bio-oil will be at low concentrations with respect to the sand/alumina. In order to accomplish this goal, the model should consider: (a) the motion of the droplets within the chaotic movement of a fluid bed (which points out to the necessity of the turbulence model that is part of Task 2 above, as well as to an appropriate drop motion model); (b) the cracking reactions that convert the bio-oil vapors into small radicals; (c) dehydrogenation/hydrogenation reactions at the Ni crystallites when and if Ni is present on the alumina-based carrier; and (d) reforming the radicals by the species resulting from the dissociation of water in the alumina surfaces surrounding the Ni crystallites. Ideally, the model should also include: (i) the inevitable propensity of specific components of the bio-oils to polymerize; (ii) the formation of coke onto the catalyst thus lowering its activity; and (iii) the partial oxidation of the coke deposits to continuously regenerate the catalyst. Obviously, it is necessary to acquire the chemical kinetics information necessary for building such a model. Jet Propulsion Laboratory will look for information on all these area in the literature, and will count on the experience of their NREL collaborators to point out to Jet Propulsion Laboratory fundamental information on these numerous items.

Biomass Pyrolysis for Hydrogen Production
Jet Propulsion Laboratory

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Code Transfer to NREL					◆	
Finalization of the Fluidized Bed Reactor, Dual Purpose Model						
Complete the turbulence model		◆				
Complete code of turbulence model				◆		
Results on the reactor evolution						◆
Modeling of the Fluidized Bed Reformer						
Literature search				★		
Model of injected-drop motion in a fluidized bed reactor		◆				
Model of injected-drop evaporation in a fluidized bed reactor			◆			
Baseline results						◆

FY 2001 Begins October 1, 2000

Hydrogen from Biomass for Use in Urban Transportation- Clark Atlantic University

Agriculture is Georgia's largest industry and contributes over \$46 billion to the state's annual economic output. One in six Georgians work in an agriculture-related sector and Georgia ranks as the number one state in the U.S. in peanut production; producing about 45 % of all peanut grown in the U. S. Georgia farmers grow about 1.5 billion pounds of peanut in 79 counties. In 1998 Georgia produced about 1.54 billion pounds (768,500 tons) of peanuts which was 15 % more than that of 1997. Disposal of the large quantity of peanut shells in an environmentally acceptable manner is a significant challenge for the peanut industry.

Biomass can be converted to hydrogen by two distinct strategies: 1) gasification followed by shift conversion and 2) fast pyrolysis followed by catalytic steam reforming and shift conversion of specific fractions. The National Renewable Energy Laboratory (NREL) technology uses the latter approach, which has the potential to be cost competitive with current commercial processes for hydrogen production. The NREL process has been demonstrated at the bench scale using model compounds. Bio-oil is easily transportable so the steam-reforming step can be carried out at a different location, close to the infrastructure for hydrogen use or distribution. This method produces two bio-oil fractions: a monomer-rich aqueous fraction (containing typically 20 wt% organics) and a hydrophobic fraction composed mainly of oligomers derived from lignin. Steam reforming can be conducted with the entire bio-oil or with each of the fractions of the oil to yield hydrogen. The remainder of the oil or biomass can be used to develop co-products, which are needed to make the hydrogen from biomass competitive with conventional sources.

This project focuses on the use of the by-products from a process for making activated carbon from densified peanut shells at Scientific Carbons Inc. in Southwest Georgia. The objective is to undertake the engineering research and pilot-scale process development studies in the use of the large quantities of peanut shells produced in Georgia as feedstock for the pyrolysis-steam reforming process to produce hydrogen for urban transportation. The project team is composed of Clark Atlanta University, Georgia Tech, Enviro-Tech Enterprises, Inc. and Scientific Carbons, Inc. NREL will work with the project team in transferring the technology.

Task 1: Feed Supply, Process Economics and Deployment

This task will develop decision models for selecting among feedstock, process and deployment alternatives. Of particular interest are peanut shells supply and cost projections and the evaluation of other agricultural residue feedstocks available in the same geographical area. Process economics will be developed for the major process options and used to construct a process options database. Different network options will be developed to determine optimum subdivision of tasks among potential sites and to develop criteria for location of new processing sites.

Task 2: Reactor Development and Commissioning

This task will design and build the reactor system which will be equipped with fluid bed reactor, vapor and liquid injection, steam injection, cyclones for disengaging catalyst particles, heat exchanger to recover heat and condense the water vapor, instrumentation and data acquisition system, and safety features. Initial shakedown of the reactor will be performed at the NREL Thermochemical Users Facility in Golden, Colorado. The steam reforming catalyst will be acquired. Initial tests will monitor catalyst fluidization, attrition and performance. After successful testing, the unit will be shipped to Scientific Carbons, Inc. for long term testing.

Task 3: Preparation for Long Term Testing at Scientific Carbons, Inc.

The design and construction of an interface will be undertaken to enable the long term testing of the reactor unit at Scientific Carbons, Inc. This will include the design, construction and addition of a slipstream capable of withdrawing 10-20 kg/h of Scientific Carbons pyrolysis vapors. The actual long-term operation of the unit will not occur in this phase (FY2001) of the project.

Task 4: Preparation for Hydrogen Storage and Utilization

Past approaches to the storage of hydrogen in mixtures with compressed natural gas will be reviewed and calculation of mixture limits will be made. Other storage options will be explored that will meet the needs of the planned demonstration. Model system testing will be performed. In preparation for hydrogen utilization, Phase 1 will include identifying the community partner and working with that partner to define the transportation fleet applications. The design of a storage system will be done.

Task 5: Environmental and Technical Evaluation

This task will design, acquire, and prepare the necessary analytical systems to optimally monitor the transportation system performance.

Task 6: Partnership Building and Outreach

This task will develop in this phase of the project relationships with community partners and the necessary memorandums of understanding (MOU) among the various parties involved in the project and its implementation

Hydrogen from Biomass for Use in Urban Transportation Clark Atlantic University						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Feed Supply, Process Economics and Development						
Develop database and optimize process options				◆		
Reactor Development and Commissioning						
Complete reactor construction			★			
Install reactor at NREL			★			
Continuous 8-hr operation of reactor				◆		
Preparation for Long Term Testing						
Complete design of interface				◆		
Preparation for Hydrogen Storage and Utilization						
Complete design of storage and utilization system				◆		
Environmental and Technical Evaluation						
Design, acquire and setup analytical system					◆	
Partnership Building and Outreach						
Complete memorandums of understanding among partners				◆		

FY 2001 Begins October 1, 2000

Supercritical Water Partial Oxidation - General Atomics

General Atomics, together with Environmental Energy Systems Inc. (EESI) and Combustion Systems, Inc. (CSI) are developing an advanced power generating system based on Supercritical Water (SCW) technology. Supercritical Water Partial Oxidation (SWPO) is a new technology for efficient and environmentally attractive and hydrogen production from low-grade fuels such as biomass, municipal/solid waste (MSW0 and high-sulfur coal).

SWPO involves carrying out oxidative reactions in the SCW environment – akin to high-pressure steam – in the presence of sub-stoichiometric quantities of an oxidant, typically pure oxygen or air. The key advantage of the proposed SWPO process is the use of partial oxidation in-situ to rapidly heat the gasification medium, resulting in less tar formation and improved hydrogen yields. Another major advantage is the high pressure, high-density aqueous environment that is ideal for reacting and gasifying organics. The high water content of the medium encourages formation of hydrogen and hydrogen-rich products. Because the process is carried out in a medium of high-pressure steam, it is highly compatible with high water content feeds, as is typical of many biomass materials. By the same token, the high water content of the medium is effective for gasification of hydrogen-poor materials such as coal. The pressurized nature of the SWPO process naturally lends itself to the liquefaction of CO₂. By combining pressure with the cold sink available from the liquid oxygen oxidant, CO₂ is readily liquefied. It may then be recycled, injected for oil recovery or otherwise handled to reduce greenhouse emissions.

Other advantages offered by SWPO include the following:

- Provides a clean fuel gas with high yields of hydrogen
- Recovers the energy required to preheat feed slurries
- Provides high-pressure effluents that can be effectively used for hydrogen separation
- Utilizes compact equipment that minimizes capital cost and footprint requirements
- Provides attractive environmental benefits, including negligible particulate, NO_x and SO_x emissions
- Produces an ash product that passes TCLP requirements for disposal or, alternatively, one that may be recycled
- Effluent gas leaves process at a low temperature and with low moisture content, so a smoke or steam plume is not present

Task 1: Bench-Scale Testing

In this task General Atomics' plans to develop a detailed test plan, including feedstock, operating conditions, process measurements and instrumentation for bench-scale tests of SWPO technology. They will also modify the existing GA-owned bench-scale equipment, perform a SWPO baseline on cornstarch which will be followed by biomass fuels and coal. An analysis will be conducted on the liquid and gaseous effluents from the bench scale tests. A test report will be produced to reduce the data from the bench-scale tests per the Test Plan, this report will include tables of the test results.

Task 2: Pilot-Scale Design and Analysis

General Atomics will prepare a pilot-scale conceptual design, Process Flow Diagram, and core process equipment, based on the results from Bench-Scale Testing. They will also prepare system engineering configuration evaluations and analytical models to evaluate overall system performance, including a comparison of the bench-scale SWPO data with prior test data and gasifier designs. Preparation of Piping and Instrumentation Drawing, equipment lists, and line sizing will be included in this task. Finally, General Atomics will prepare interface specification, utility requirements and operating cycle analysis.

Task 3: Development Plan

General Atomics will prepare a SWPO development plan, including cost and schedule estimates; define the follow-on technical development plan and business development plan required for the complete, multi-phase development of the SWPO concept. A pilot scale demonstration will be conducted by developing unit operations tests of core-process equipment, followed by and integrated demonstration with other pilot-scale operations for hydrogen separation and storage. A business plan and proposal will be prepared to identify SWPO market potential, including economic analyses relative to other hydrogen generation methods; define follow-on activities from bench-scale testing through pilot-scale demonstration of an integrated SWPO system, including follow-on proposal.

Task 4: Project Management

General Atomics will coordinate the team members to meet project goals within scope, schedule and cost constraints.

Phase 2 – Technology Development

This work is anticipated to include scale-up and testing of a pilot-scale SWPO reactor to resolve knowledge gaps and other critical issues, and to define performance requirements and system interfaces for the subsequent Phase 3 System Integration and Design effort. Phase 2 is anticipated to start in June 2001.

Supercritical Water Partial Oxidation General Atomics						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Bench Scale Tests						
Issue test plan		◆				
Equipment ready for test			◆			
Complete Bench Scale SWPO Testing			★			
Receive analysis				◆		
Issue test report				◆		
Pilot Scale Design						
Issue design basis				◆		
Complete process design				◆		
Finalize system design				◆		
Identify facility requirements				◆		
Development Plan						
Issue development plan				◆		
Complete demonstration plan				◆		
Submit business plan and proposal				◆		
FY 2001 Begins October 1, 2000						

Biohydrogen Production from Renewable Organic Wastes – Iowa State University

For global environmental considerations, production of hydrogen by biological reactions, from renewable organic waste sources represents an important area of bioenergy production. Many investigations have been conducted using pure cultures of hydrogen-producing bacteria. Some of the studies showed promising results. However, since wastewater is contaminated by bacterial, the purity of any wastewater treatment reactor is lost and therefore the treatment of wastewater has to be a mixed culture process. Moreover, these studies were limited to the basic studies on microbial hydrogen metabolism. Their viability to real processes in terms of technical feasibility and commercialization potential has not been evaluated. The goal of this project is to develop an anaerobic fermentation process that converts negative value organic wastes into hydrogen-rich gas that can significantly enhance the economic viability of many processes either by utilizing hydrogen as a fuel source or as raw material for industries that consume hydrogen. The project will contribute to the U.S. DOE's goal of "producing hydrogen from renewable energy resources at a cost of \$10 -\$15 per million BTU for direct renewable systems without significant carbon dioxide emissions."

In this research project, fundamental and practical feasibility studies of hydrogen fermentation from negative value organic wastes will be conducted using naturally available inocula (i.e., natural and compost) in continuous flow bioreactors. Various selection pressures will be used to minimize contamination of the hydrogen-producing bacterial culture and avoid undesirable by-products. By selecting suitable waste streams and providing a favorable environment for the hydrogen-producers, relatively high conversion efficiencies will be maintained.

Task 1: Optimization of Hydrogen Production with Synthetic Wastes

The task will be a lab-scale investigation of the operational protocols for hydrogen production and waste stabilization. This fundamental study will use synthetic carbohydrate-rich wastes that mimic actual industrial or agricultural wastes. This will allow the researchers to control the system operating environment and characterize the microbial communities that produce hydrogen gas better. Two parallel anaerobic chemostat fermenters will be operated at a mesophilic temperature in the project.

Subtask 1-1: Enrichment of Mesophilic Hydrogen-producing Microorganisms

Secondary anaerobic digested or hydrogen-producing microorganisms from natural resources as tested in the preliminary experiment will be used as inocula for this research. A heat pretreatment process will be performed on the inoculum to inhibit the biological activity of hydrogen-consumers in the anaerobic sludge seed. At least some mesophilic hydrogen-producing microorganisms are spore forming bacteria (e.g., *Clostridium* sp.) and therefore should survive heat treatment. Thus, these microorganisms will be enriched in the inoculum. The inoculum will be further cultivated in the chemostat fermenters with a carbohydrate-rich substrate. After the cultivation period, the organic loading of the reactor will be increased to conduct the next step of the research.

Subtask 1-2: Influence of pH, Temperature, and Mixing Intensity

Two environment-controlled fermenters will be used for this stage of the study. These fermenters will be loaded at a constant organic loading rate of 6 g COD/L/day and tested at different operating pH, temperatures, and mixing intensities (rpm) of the mixer. The proposed operating pH is 4.0, 5.0, 6.0, and 7.0 and the proposed operating temperatures are 25, 30, 35, and 40 °C.

Task 2: Microbial Community Characterization

The microbial community structure of the biomass samples collected from bioreactors with various operating conditions will be characterized using a top-to-bottom approach with quantitative membrane hybridizations. In brief, RNA will be extracted from samples with a low-pH hot-phenol bead-beating procedure. RNA will be immobilized on nylon membranes and hybridized with oligonucleotide probes radiolabeled with ^{32}P . Hybridization signals will be quantified using an InstantImager[®] Electronic Autoradiography System from Packard Instrument Company (Meriden, CT). A set of previously developed oligonucleotide probes will be used first. Subsequently, new, more specific probes will be developed to quantify specific hydrogen-producing populations.

Task 3: Process Optimization of a Continuous-Flow Reactor

Two additional lab-scale bioreactors will be operated as completely stirred tank reactors. They will be operated at different organic loading rates by controlling the hydraulic retention time (HRT) with the optimal pH and temperature determined in the previous step. The F/M ratio, an important parameter, will also be manipulated by wastage of sludge from the reactors at regular intervals. The mixer rpm will be controlled at the optimum velocity for immediate removal of the produced hydrogen gas from the system. The experience from this study will provide valuable information to establish design criteria for a pilot-scale reactor degrading real wastes.

Task 4: Investigation of Hydrogen Production Potential of Different Wastewaters

Batch experiments using serum bottles will be conducted to test the hydrogen production potential of different wastes. This will provide a preliminary assessment of the hydrogen production potential of the various waste streams. The results from this task will assist in the selection of potential target waste streams for the production of hydrogen. The microflora isolated during the previous task will be used as inoculum for this stage. The waste streams that will be tested during this stage of the study will include food processing wastewater (potato and whey), agricultural residuals such as corn stalks, municipal wastes, industrial wastes, pulp and paper wastes, and meat packing wastes.

Task 5: Pilot Test of Selected Waste Streams

Pilot test will be conducted on the potential waste streams identified from Task 4.

Biohydrogen Production from Renewable Organic Wastes Iowa State University						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Optimization of H₂ Production with Synthetic Wastes						
Enrichment of mesophilic H ₂ -producing microorganisms	◆					
Influence of pH, temperature, and mixing intensity		◆				
Microbial Community Characterization					◆	
Develop detailed process flow sheet						
Process Optimization of a Continuous-flow Reactor				★		
Investigation of H₂ Production Potential of Different Wastewaters					◆	
Pilot Test of Selected Waste Streams						◆

FY 2001 Begins October 1, 2000

Bio-production of Hydrogen using Thermophilic Bacteria - National Energy Technology Laboratory

This project continues ongoing investigations related to the biological production of hydrogen by extremophilic bacteria. To date, over 3,900 samples have been examined. The National Energy Technology Laboratory (NETL) has demonstrated that in a batch type experiment they can produce up to 13.1 ml hydrogen/50 ml of culture medium in 22 hours of incubation. This is calculated to be an average rate of 11.91ml/liter-hr. In these same batch-type experiments accumulations of up to 34% hydrogen have been readily observed. Moderate levels of oxygen do not seem to inhibit this process, as up to 15% oxygen is readily tolerated.

NETL is currently beginning continuous culture experiments using these extremophiles. To date, they have been able to generate produce hydrogen at a cumulative efficiency of up to 5.58 % hydrogen gas for 2 liter cultures for periods of several weeks. It is apparent even from these initial studies that factors such as pH, amount and type of sulphur-containing compounds, substrate type and availability can greatly affect the hydrogen yield. NETL is cautiously optimistic that this process can be scaled up to efficiently yield significant amounts of hydrogen, and thus, the objective of this study is to determine if the process can indeed be scaled up.

This project is designed to address the nation's increasing emphasis and demand for cost-effective production of hydrogen as an ultraclean fuel for the future. NETL has surveyed thermophilic bacteria of the order *Thermotogales*, and have found that they are excellent organisms for effectively utilizing organic waste materials and producing hydrogen gas biologically. NETL has demonstrated that all bacteria of the order *Thermotogales* produce hydrogen, and this is likely to be a hitherto unrecognized characteristic of the order. In FY 2001 NETL will concentrate on optimizing the use of *Thermotoga neapolitana* for biohydrogen production.

Task 1: Continue to Refine and Utilize Systems Analysis to Predict Commercial Potential

Commercial applicability is the long-term goal of this project, so NETL has begun work to assess this. The systems analyses will involve all aspects of the system: capital costs, start up, maintenance, and operations.

Accuracy of the systems analysis will depend on conducting complete biochemical analysis and control of the bio-hydrogen generation process. Thus, the balance of the work goals for FY01 will involve development of a clear understanding of the biochemical processes occurring during the process. These biochemical goals are stated below.

Task 2: Complete Identification of Best Performing Strain for Fermenter Utilization and Potential Scale-Up

Thermotoga neapolitana, *Thermosipho* sp., and *Fervidobacterium pennavorans* have been found to be the most productive strains of bacteria tested to date. More complete testing and comparison of these three strains will be undertaken using fermenter technology to compare the maximum rate and length of time for which steady-state production rates are attainable.

Task 3: Determine How Long The Reactor Can Be Made To Run At Steady-State Before Hydrogen Yield Decreases to Inefficient Levels

The preliminary data suggests that the reactor will show a massive increase in biomass within the first day of incubation. During this growing (log) phase, little hydrogen is produced. As the cells enter the stationary phase, when no growth occurs but the cells are still actively metabolizing, a high yield of hydrogen is seen. From the start of incubation to the time when hydrogen yield first begins to decrease is approximately 5-6 days. We have observed that production can again be stimulated by sparging the system with nitrogen gas to remove excess hydrogen sulfide. Hydrogen gas production will then increase for a period of about 24 hours. After several days of doing this, even intermittent sparging is unproductive.

Task 4: Determine why the Hydrogen Yield Decreases

This is considered the most crucial goal for FY01. Several possibilities exist here, the most likely are listed below and investigation of each of them will be the basis for much of the work conducted this year .

a. The substrate could be used up by the phenomenal increase in bacterial mass.

An accurate stoichiometric ratios of biomass, product gases, will be obtained. NETL has recently purchased a liquid chromatograph specifically designed for biological use (BioLC) and will use this to determine the amount of substrate (carbohydrate, food) remaining in the solution.

b. The hydrogen sulfide produced when sulfur is released from the cysteine added to the medium to promote more rapid bacterial growth inhibits the reaction.

As stated above, sparging for 15 minutes to remove hydrogen sulfide gas buildup in the fermenter results in increased hydrogen gas production, so we suspect that indeed reduced or free sulfur in the medium affects continuous hydrogen gas generation. NETL will more closely address the role of free or reduced sulfur compounds in this process with the goal of finding a substitute for the sulfur that will promote (or not inhibit) growth. Concomitantly, NETL will be attempting to reduce the generation of hydrogen sulfide gas by the bacteria.

c. An inhibitory end-product could be building up in the medium that needs to be identified and removed.

NETL will utilize their newly purchased BioLC to identify putative catabolites that build up with prolonged incubation and approximate the concentrations at which they become inhibitory to the system. They will then determine how to most effectively reduce the catabolites in the growth medium.

Task 5. Continue to Explore Potential Commercial Contacts

It is anticipated that most of the work necessary to develop this product will be completed within the next three years. With that goal in mind, we will be networking to establish commercial partners for this technology.

Bio-production of Hydrogen using Thermophilic Bacteria
National Energy Technology Laboratory

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Continue to refine and utilize systems analysis to predict commercial potential					◆	
Complete identification of best performing strain for fermenter utilization and potential scale-up		◆				
Determine how long the reactor can be made to run at steady-state before hydrogen yield decreases to inefficient levels			◆			
Determine why the hydrogen yield decreases				◆		
Continue to explore potential commercial contacts					◆	

FY 2001 Begins October 1, 2000

Critical milestone is to be determined

Biological H₂ from Fuel Gases and from Water – National Renewable Energy Laboratory

An economic process for producing H₂, biologically or chemically based, would ideally be H₂O derived, solar driven, highly efficient, durable, insensitive to H₂ partial pressure, and inexpensive to build and operate. Of the biological options, systems of intact cells of photosynthetic bacteria are the most advanced. Unlike cyanobacteria or algae, photosynthetic bacteria do not oxidize H₂O and do not directly fulfill the first criterion. They do, however, evolve H₂ from biomass (previously generated from sunlight, H₂O, and CO₂). These bacteria use several different enzymatic mechanisms with near-term commercial potential for biological H₂ production from biomass. One mechanism in particular looks promising for applications as a biological conditioning agent for upgrading thermally generated fuel gases to a level where they can be directly injected into hydrogen fuel cells. This same system has potential to subsequently evolve into a second-generation photobiological method to produce H₂ from H₂O, potentially fulfilling all of the ideal system requirements.

The near-term project goal is to investigate and optimize the microbes and conditions that enhance bacterial fuel gas conditioning for H₂ production. A mid-term goal is to create a transgenic cyanobacterial strain containing an O₂-tolerant bacterial hydrogenase that will simultaneously evolve H₂ and O₂ from H₂O.

A unique type of hydrogen-producing activity was found in a strain of photosynthetic bacteria that functioned only in darkness to shift CO (and H₂O) into H₂ (and CO₂). NREL has since isolated more than 400 strains of photosynthetic bacteria from local sites that perform this shift reaction in darkness, and will also quantitatively assimilate CO into new cell mass in light. The terminal CO-linked hydrogenase functions preferentially in the evolution direction and exhibits high degree of O₂ tolerance. NREL has demonstrated the existence of at least three separate hydrogenases in *Rhodospirillum rubrum*: they are CO-linked, formate-linked, and uptake hydrogenases. In order to quantify the O₂ tolerance of the hydrogenase of interest without complications from others, NREL has devised conditions where only the hydrogenase of interest is selectively induced through manipulations of cell physiology, biochemical purification and genetic studies. Using fractions enriched in only the CO-linked hydrogenase and measuring the D₂O-H₂ exchange activity, NREL determined that CO-linked hydrogenase is still partially active (60%) even when it is stirred in 13% of O₂ for 20 min. More than 90% of the activity is recovered upon the subsequent removal of O₂. NREL has since identified proper instrumentation and assay conditions that will allow for the kinetic measurement of H₂ evolution upon O₂ additions.

NREL's ability to induce each hydrogenase separately also enables them to determine the electron acceptor/mediator each enzyme can use. All three hydrogenases can use the low-redox mediator methyl viologen in both the forward and backward directions. However, only the uptake hydrogenase can use the high-redox dye methylene blue. NREL has, therefore, developed unique assays allowing them to monitor each hydrogenase specifically, which will aid in the further purification of the CO-linked hydrogenase.

NREL have successfully isolated a mutant deficient in the hydrogen uptake pathway (HUP) based on its conditional sensitivity to photo-oxidative killing conditions. Using the same scheme, they have attempted to isolate mutants deficient in various components of the CO to H₂ pathway. NREL has identified that the rate-limiting step for getting a mutant is the slow growth of colonies on agar plates under an atmosphere of CO. They are exploring other enrichment/selection schemes to facilitate mutant isolation.

Microbiology research focuses on two different, but related, tasks. The near-term task (Task 1) is designed to characterize the bacterial water-gas shift reaction at biochemical and genetic levels so that it can be further enhanced in both activity and stability of hydrogen production from thermally gasified

biomass at PDU-scale levels. The longer-term task (Task 2) will exploit the genes that code for the special evolving hydrogenases from bacteria that have been isolated and bred to be oxygen resistant, and genetically transfer the genes coding the necessary proteins to a cyanobacterial host where they can function in the simultaneous photogeneration of hydrogen and oxygen from water.

Task 1: H₂ from Biomass

NREL will develop protocols to completely purify the CO dehydrogenase and O₂-tolerant hydrogenase, enzymes and identify methods such as embedding in synthetic micelles and liposomes to enhance its stability. Compositional analysis and amino acid sequence can be derived from the purified protein. Based on the amino acid sequence, NREL will be able to design more specific DNA or RNA probes to aid in the cloning of the hydrogenase gene for Task 2. Characterization of the purified hydrogenase will elucidate the electron mediators to which it can couple, which helps determine if the hydrogenase will use the photoreductants generated from the water-splitting reaction of a cyanobacterium. A purified hydrogenase enzyme can also be examined for its oxygen resistance without any qualifications about possible contaminant activity. Collaboration with European scientists to determine the three-dimensional structure of the O₂-tolerant hydrogenase is being discussed and would provide enormous insight into the nature of O₂-tolerance.

Through differential detergent extractions, NREL will obtain fractions enriched in the electron-mediating cofactor involved in the linked pathway. They will attempt to develop a unique assay for this cofactor. The identification of this cofactor will also aid in meeting NREL's goal of transforming a cyanobacterium with the bacterial hydrogenase system (Task 2), as it may be necessary to transfer this cofactor also along with hydrogenase in order to mediate electron transfer from water oxidation to H₂ production.

NREL will continue to develop other selection and enrichment schemes based on the ability of CO oxidation either generating CO₂ as a required substrate for growth, or its reduction of methyl viologen as a color indicator. A complete library of such mutants will be generated encompassing all encoded proteins in the CO-linked pathway. Constitutively over-expressed, water-gas shift mutants will be sought by examining their revertants. This will promote maximal specific CO shift rates.

Task 2: H₂ from Water

NREL will continue to utilize a capillary mass spectrometer to obtain kinetic data of both activity and durability of H₂ production with various levels of O₂ simultaneously present. This system introduces samples to the detector continuously at ambient pressure via a capillary leak. Since a carrier gas is not required, no sample dilution occurs. NREL will perform measurements with both whole cells and purified hydrogenase enzyme obtained from Task 1. Characterization of the purified hydrogenase will determine if O₂-tolerance is an intrinsic property of the nature of the protein, and not owing to high respiratory activities of whole cells.

NREL will develop molecular biological techniques construct the cyanobacterial-bacterial hybrid. NREL will induce CO oxidation systems with the addition of CO to a photosynthetic bacterial culture and isolate total RNA. The presence of a CO-induced hydrogenase transcript can be determined qualitatively via Northern blot technique using a DNA probe. A specific DNA probe can be constructed according to amino acid sequence analysis of the purified hydrogenase from Task 1. This is the preferred choice. Alternatively, NREL would design a DNA probe based on homologous regions of related hydrogenase of known gene sequence. Using RT-PCR and random primers, a cDNA library can be constructed from the RNA pools to include those DNA sequences originated from mRNA induced only upon CO addition.

The cDNA library will be screened for those recombinant clones containing the genes of interest by colony hybridization assays using a ^{32}P -labeled DNA probe. Those clones carrying the hydrogenase gene will be amplified with PCR to determine if they indeed contain the correct DNA sequence coding for a hydrogenase protein.

Biological H₂ from Fuel Gases and from Water National Renewable Energy Laboratory						
Task Designation/Milestone		2001				2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Hydrogen from Biomass						
Improve the purification of hydrogenase					★	
Hydrogen from Water						
Link O ₂ -tolerant hydrogenase to photoreductants generated from cyanobacteria in a mixed extract					◆	
FY 2001 Begins October 1, 2000						

Bioreactor Development For Biological H₂ Production – National Renewable Energy Laboratory

A large number of bacterial strains have been isolated that perform the water-gas shift reaction on syngas ($\text{CO} + \text{H}_2\text{O} = \text{H}_2 + \text{CO}_2$). At biological temperatures ($<50^\circ\text{C}$), the equilibrium constant for the shift reaction is in excess of 30,000, ensuring that the biologically catalyzed reaction can readily approach completion with little residual CO. The bacteria can also oxidize H_2S and COS from gas streams. The conditioned product gas is sufficiently clean for direct injection into PEM or phosphoric acid fuel cells.

The near-term project goals are to develop bioreactors with enhanced mass transfer capabilities that will promote an economic biological process for conditioning of fuel gases for direct use in fuel cells, and to demonstrate the water-gas shift reaction on syngas produced from steam reforming of natural gas and biomass gasification.

Previous work has indicated that mass transfer of gaseous CO into the aqueous phase is the rate-limiting step of the process. The present focus of the work is on the development of improved bioreactor designs, and on collecting performance data using syngas streams produced by steam reforming and biomass gasification.

In the previous year NREL has demonstrated convincingly that the microbiological water-gas shift reaction is limited by the rate of gas transfer into the culture media. In this respect, the water-gas shift reaction is like most aerobic biological processes, in which oxygen transfer to the liquid phase is limiting the overall rate. Such limitations in aerobic biological processes are successfully addressed by selecting the appropriate bioreactor design, and NREL is approaching the mass transfer issue in the water-gas shift reaction in the same way. NREL has tested a number of reactor designs and have collected promising rate data from both trickle bed and bubble-column bioreactor designs.

NREL has also developed a computer-controlled research/demonstration skid that consists of a steam generator and a catalytic reformer to produce a “real-world” synthesis gas mixture ready for biological conditioning. A near-infrared (NIR) CO monitor is used to measure and regulate the syngas flow to maintain less than 10 ppm residual CO in the conditioned gas. A 50W PEM fuel cell completes the assembly.

Bioreactor development work is divided into two different tasks. The first task involves the development of an optimum bioreactor design, while the second task combines syngas production with microbial water-gas shift to demonstrate the cleanup of “real-world” syngas.

Task 1: Bioreactor Design and Scale-Up

NREL tested bubble column reactors and trickle bed bioreactors with different internal packings in reactor loops with liquid culture volumes up to 1 liter, and these results are very encouraging. In FY01, NREL will continue their reactor scale-up activities. A goal has been set to increase the size of the bioreactor 5-fold, as measured by the culture volume.

Task 2: Syngas Production/Cleanup

In a real-world application, syngas will be supplied to the bioreactor either by reforming a gaseous or liquid hydrocarbon fuel, or by biomass gasification. The syngas produced by either of these processes will contain other species besides CO and H_2 . For example, syngas produced by natural gas reforming will

likely contain uncracked propane and other hydrocarbons, while syngas from biomass gasification can contain ash, tar, and trace amounts of aromatics. NREL's computer-controlled research/demonstration skid can produce syngas from natural gas or propane reforming, and can be modified to include a small biomass gasifier.

In FY 2001, NREL will examine the effect of trace species present in synthesis gas derived from the gasification of biomass by operating a bioreactor with synthesis gas produced from biomass gasification.

Bioreactor Development for Biological H₂ Production National Renewable Energy Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Bioreactor Design and Scaleup						
Demonstrate scaled-up bioreactor using a liquid media volume of 5 liters					◆	
Syngas Production/Cleanup						
Operate bioreactor to condition biomass-derived synthesis gas					★	
FY 2001 Begins October 1, 2000						

SEPARATION AND PURIFICATION

Separation Membrane Development - Westinghouse Savannah River Technology Center

The goal of this project is to develop an energy efficient hydrogen separation process based on a new class of composite materials. This new separation process will resist harmful impurities in the feed stream such as oxygen and carbon monoxide, and will be energy efficient. The approach that will be investigated is a thermal absorption process using sol-gel encapsulated metal hydride material. It is known that metal hydrides absorb hydrogen reversibly and can be used to separate hydrogen from other gases. The problem with metal hydrides is that they can be poisoned by impurities such as oxygen and carbon monoxide. Earlier work at the Savannah River Technology Center (SRTC) has showed that using a sol-gel process, metal hydride particles can be encapsulated in a highly porous silica matrix. The porosity can be controlled so that the pores permit hydrogen to reach the metal hydride but prevent the larger molecule impurities such as oxygen and carbon monoxide from poisoning the reactivity of the metal hydride. These results indicate that a hydrogen separation column can be produced using the encapsulated metal hydride particles. This column will absorb hydrogen from a gas mixture when it is cooled and will release the absorbed hydrogen when it is heated to produce a high purity hydrogen stream.

The largest volume of hydrogen produced today (> 90%) is produced at the point of use by petroleum refineries and ammonia manufacturers. Discussion with major US companies in both of these two industries indicates significant interest in SRTC hydrogen separation and recovery technology. Applications of SRTC sol-gel, metal hydride technology to smaller stationary and onboard partial oxidation (POX) systems as well as to the recovery of hydrogen from biomass derived fuels are also being investigated.

Task 1: Produce Hundred-gram Size Sample

A key objective for FY-01 is to evaluate the hydrogen separation property of a packed column using Sol-gel encapsulated metal hydride. To accomplish this objective, hundred-gram size samples of sol-gel encapsulated metal hydride must first be produced. Earlier work has been concentrated on making gram-size samples. The experience accumulated in making these small samples need to be reviewed and scale-up procedure defined to produce larger samples. The following subtasks are identified:

- Review past experience
- Define scale-up procedure
- Produce large samples
- Reiterate to improve if necessary

Task 2 Hydrogen Separation Test

This hydrogen separation concept involves the use of a packed column. The packing material will be the sol-gel encapsulated metal hydride. The column will be thermally cycled, so that hydrogen in a gas mixture is absorbed during the cooled half-cycle and the absorbed hydrogen is released during the heated half-cycle. A laboratory scale column will be fabricated. A gas manifold will be set up to permit the evaluation of the column for hydrogen recovery from gas mixtures. The following subtasks are identified:

- Design column and manifold
- Procure components
- Fabricate column and manifold
- Conduct separation tests on hydrogen nitrogen mixture
- Conduct separation tests on hydrogen and carbon monoxide

Separation Membrane Development
Westinghouse Savannah River Technology Center

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Produce Hundred-gram Sample size						
Review past experience		◆				
Define scale-up procedure		◆				
Produce large samples			◆			
Reiterate to improve if necessary				◆		
Hydrogen Separation Test						
Design column and manifold		◆				
Procure components			◆			
Fabricate columns and manifold				★		
Conduct separation test on H ₂ /N ₂						◆
Conduct separation tests on H ₂ /CO						◆

FY 2001 Begins October 1, 2000

Defect-Free Thin Film Membranes For H₂ Separation And Isolation – Sandia National Laboratories

This project focuses on the research and development of crystalline, inorganic, molecular sieve (zeolite) thin film membranes for light gas molecule separations. In particular, SNL is interested in separating and isolating H₂ from CH₄, CO and N₂ gases. Current hydrogen separation membranes are based on Pd alloys or on chemically and mechanically unstable organic polymer membranes. The use of molecular sieves brings a stable (chemically and mechanically stable) inorganic matrix to the membrane. The crystalline frameworks have “tunable” pores that are capable of size exclusion separations. SNL envisions the impact of positive results from this program in the near term with Hydrocarbon fuels, and long term with Biomass fuels.

SNL will work on synthesis, modeling and thin film growth of novel microporous phases for light gas separations, including novel gallo phosphates and silicotitanate phases. Furthermore, SNL will explore the thin film growth of aluminosilicates zeolites doped with other elements for maximized adsorption and selectivity of H₂ over other light gases of interest. SNL will also begin to build interactions and collaborations with outside industries for potential future collaborations and commercialization partnerships.

Task 1: Thin Film and Bulk Growth

This task involves growth of aluminosilicate (Al/Si) zeolite thin films (such as Faujasite) doped with other elements for light gas separations. As well as synthesis of defect-free gallophosphate (Ga/P) and silicotitanate (Si/Ti) phases as thin film membranes (with 100% coverage, <50μm thick), synthesis and characterization of bulk microporous alkali gallophosphate (Ga/P) phases, and synthesis of bulk phosphate and titanate novel phases. Finally SNL will characterize all new phases (X-ray diffraction, thermal analyses, surface area, and elemental analysis).

Task 2: Modeling and Simulation

This involves modeling separation values by molecular dynamics calculations for both pure light gases interacting with the novel Ga/P, Al/Si and Si/Ti frameworks and mixtures of light gases interacting with the novel Ga/P, Al/Si and Si/Ti frameworks.

Task 3: Permeation Studies

Permeation studies of pure gases through membranes and mixture gases through membranes.

Task 4: Business Development

Initiate a Commerce Business Daily announcement as a first step in finding a CRADA partner. (An example might be working with an industrial partner in membrane development.)

Defect-Free Thin Film Membranes for H₂ Separation and Isolation
Sandia National Laboratories

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Thin Film and Bulk Growth of Inorganic Porous Materials						
Al/Si film Growth				◆		
Ga/P and Si/Ti Film Growth				◆		
Bulk Ga/P new phases		◆				
Bulk phosphate and titanate based phases					◆	
Modeling and Simulation						
Pure gases				◆		
Mixture gases					◆	
Permeation Studies						
Permeation of pure gases through membranes					★	
Permeation of mixture gases through membranes						★
Business Development						
Initiate Commerce Business Daily					★	

FY 2001 Begins October 1, 2000

Table 3.2 Renewable Production		
Goal: Advance emission-free, and renewable-based hydrogen production technologies towards commercial viability, with a target cost of \$10-\$15/MMBtu.		
Category	Project	Researcher
<i>Electrolytic Processes</i>	Solar Photocatalytic H ₂ Production from Water using a Dual Bed Photosystem	Florida Solar Energy Center
	Photoelectrochemical Based Direct Conversion for Hydrogen Production	National Renewable Energy Laboratory
	Photoelectrochemical Hydrogen Production	University of Hawaii
<i>Photobiological Processes</i>	Development of an Efficient Algal H ₂ – Production System	National Renewable Energy Laboratory
	Hydrogen Production by Photosynthetic Water Splitting	Oak Ridge National Laboratory
	Maximizing Photosynthetic Efficiencies and Hydrogen Production by Microalgal Cultures	University of California, Berkeley
	A Cyclic Photobiological Algal Hydrogen Production System	National Renewable Energy Laboratory
	International Energy Agency and Other International Collaborations	National Renewable Energy Laboratory
	Efficient Hydrogen Production Using Enzymes of the Pentose Phosphate Cycle	Oak Ridge National Laboratory

ELECTROLYTIC PROCESSES

Solar Photocatalytic H₂ Production from Water Using a Dual Bed Photosystem - Florida Solar Energy Center

Photocatalytic compounds in particulate form are being employed in various dual modular configurations so as to effect the solar-driven decomposition of water to its constituent elements, particularly hydrogen. The system advantages are low manufacturing cost, safe evolution of H₂ and O₂ in separate compartments, and more efficient use of the solar spectrum.

Each module has its own distinctive photocatalyst according to whether it is to evolve H₂ or O₂. Earlier studies concentrated on conventional inorganic semiconductor materials. It was eventually realized that new photocatalytic materials needed to be developed to avoid lifetime problems due to corrosion and to absorb lower energy photons. A combination of semi-empirical molecular orbital calculations and voltammetric, UV-visible spectroscopic, and UV photoelectron analysis identified several organic pigment families as promising materials. These materials were tested as to their respective O₂- and H₂-evolving ability. A perylene diimide gave the best results for O₂ evolution, while copper phthalocyanine proved best for H₂ evolution.

Task 1: System/configuration Modeling

Florida Solar Energy Center's (FSEC) system calculations based on materials costs indicate that if an 8% solar to hydrogen conversion efficiency could be obtained, the resulting H₂ would sell for \$13/mbtu. To achieve this efficiency, it is anticipated that a combination of photocatalyst materials and system configuration development will be necessary. The effect of various module designs can be estimated by modeling calculations.

Subtask 1-1: Dual planar modules

Mass transport considerations would indicate that there will be a redox mediator concentration gradient across the face of each module, so that the rate of water-splitting would fall in the direction of flow of the working fluid. Diffusion and forced flow calculations will be performed to correlate the movement of the redox mediator to the module performance.

Subtask 1-2: Tandem module

One trade-off in employing dual modules or any tandem systems is that the quantum efficiency of the water-splitting process is automatically halved. This is justified by being able to utilize more of the solar spectrum. An approach successfully exploited in the photoelectrochemical area is to use tandem electrodes, that is, semiconductor electrodes made from dissimilar lamina that complement each other in terms of their electronic characteristics. It is possible to formulate a photocatalytic version of the dual bed by conceptually folding one module underneath the other. Modeling the use of tandem modules should provide a basis of comparison to the series planar arrangement.

Subtask 1-3: Perforated tandem module

In this modification, FSEC will consider whether perforating the photoactive surface to enable mediator flow from front to back through the supporting membrane, as opposed to transverse flow around it, will reduce mass transport difficulties.

Subtask 1-3: Redox conformation effect

One obvious deficiency of the photocatalytic approach to water-splitting is that little provision exists for preventing the reverse reaction, i.e., the consumption of H₂ and O₂ inside the module via reaction with the respective form of the redox mediator. It may be possible to prevent the back reaction by employing redox mediators that undergo conformational change due to change in oxidation state. The effect of reversible and irreversible mediator kinetics will be including into the modeling calculations.

Task 2: Continued Photocatalyst Development**Subtask 2-1: O₂-evolving photocatalyst**

For O₂ evolution, derivatization of the imide moiety on the perylene diimide is expected to improve its photocatalytic performance.

Subtask 2-2: H₂-evolving photocatalyst

The work done on phthalocyanines will be expanded to include other pigment families.

Task 3: Module Construction**Subtask 3-1: Photocatalyst and co-catalyst distribution**

It seems clear that co-catalysts must be included to promote acceptable charge transfer rates. The means of applying a 1.0 weight percent co-catalyst uniformly distributed over a large photocatalyst deposit area is a technique that must be developed.

Subtask 3-2: Testing under solar simulator

This will be the critical milestone, to construct a module and test it under solar simulated illumination.

Solar Photocatalytic H ₂ Production from Water Using a Dual Bed Photosystem Florida Solar Energy Center						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
System/configuration Modeling						
Dual planar modules	◆					
Tandem module		◆				
Perforated tandem module			◆			
Redox conformation effect				◆		
Continued Photocatalyst Development						
O ₂ -evolving photocatalyst		◆				
H ₂ -evolving photocatalyst			◆			
Module Construction						
Photocatalyst and co-catalyst distribution				◆		
Testing under solar simulator				★		
Participation in IEA Annex 14 Activities						
Attend fall '00 experts meeting	◆					
Attend spring '01 experts meeting			◆			
Attend fall '01 experts meeting					◆	
FY 2001 Begins October 1, 2000						

Task 4: Participation in IEA Annex activities

The former “Photoproduction of Hydrogen” Annex 10 agreement of the International Energy Agency has been reconstituted as Annex 14 on “Photoelectrolytic Production of Hydrogen.” Investigators from Switzerland and Japan that formed collaborations with FSEC during the previous agreement will be participating again in the new annex, so that it is expected that those interactions will continue. The specific interaction is under negotiation at this point, but it is anticipated that common ground will be found with the use of FSECs pigments in dye-sensitization systems.

Photoelectrochemical Based Direct Conversion for Hydrogen Production – National Renewable Energy Laboratory

A photoelectrochemical (PEC) system that uses sunlight to produce hydrogen from water consists of a semiconductor electrode in contact with an aqueous electrolyte. When a semiconductor of the proper characteristics is irradiated with sunlight, the energy is sufficient to split water into hydrogen and oxygen. The advantages of a direct conversion hydrogen generation system are that 1) it eliminates most of the costs of the electrolyzer, and 2) it has the possibility of increasing the overall efficiency of the process due to a lower current density. For direct photoelectrochemical decomposition of water to occur, several key criteria of the semiconductor must be met. The semiconductors band gap must be sufficient enough to split water ($\sim 1.7\text{eV}$), the semiconductor band edges must span both the redox potentials of the hydrogen and oxygen evolution reactions, and finally the charge transfer from the surface of the semiconductor must be fast enough to not only prevent corrosion but also reduce or eliminate band edge migration.

More advanced technologies for PEC water splitting include photovoltaic tandem cells. This technology connects two photovoltaic layers (p-n junctions) with different semiconductor band gaps in series, one behind the other in a single monolithic device. This arrangement provides the highest theoretical conversion efficiency of any photoconversion system. The combination of lower cost and high efficiency represents an important area of research.

The goal of this research is to develop a stable, cost effective, photoelectrochemical based system that splits water upon illumination, producing hydrogen and oxygen directly, using sunlight as the only energy input. Theoretical efficiency for tandem junction systems is 42%; practical III-V systems could achieve 18-24% efficiency, low cost multi-junction amorphous silicon systems could achieve 7-12% efficiency.

NRELs study of PEC direct conversion systems involves two areas of basic research: semiconducting materials, and surface treatments. Semiconducting materials can be divided into two types based on their solid state structure: single photon absorbers and multi-photon (multi-junction) devices. Surface treatments involve coatings to address energetic stability under illumination, catalysts for the water splitting reactions and corrosion problems. NRELs work on semiconductors is primarily focused on multiple photon devices; for surface treatments, their focus is on stabilizing the interface energetically, and against corrosion.

For multi-junction systems, NREL is studying: III-V semiconducting materials (materials are made with various combinations of gallium, indium, arsenic nitrogen and phosphorous); and amorphous silicon based systems. The III-V tandem cell structures are the semiconductors that solid state research groups are focusing on as the next generation of high efficiency ($>25\%$) solar cells. The amorphous silicon (a-Si) systems represent a low cost (albeit lower efficiency) silicon-based direct conversion system.

Part of this project is directed at identifying new semiconductors with suitable properties for PEC water splitting, and determining proper surface treatments to enhance reaction rates, and stabilize the surface. The a-Si/a-SiC system has also shown promise as a water splitting system. Aspects of this work have generated industrial interest.

Task 1: High Efficiency Tandem Cell and New Material Characterization

Efforts will continue to identify and understand the factors that limit the efficiency and lifetime of NRELs photoelectrochemical cell. Continuing research will also study the corrosion mechanisms and possible passivating techniques.

As part of NREL's search for semiconductor materials with inherently greater stability, they have initiated a study of nitride materials. NREL will be looking for industrial partners to grow samples of GaN and $\text{In}_x\text{Ga}_{1-x}\text{N}$ for them tailored to their specific requirements.

Identification of solution compositions and additives that stabilize the semiconductor/electrolyte interface will be critical if a more stable PEC-based, water-splitting system is to be developed. The present study is focused on the stability of the p-GaInP₂ electrode in aqueous electrolytes of different pHs. Of particular interest is the electrochemical behavior of the illuminated electrode under both open-circuit conditions and cathodic polarization. Investigation of the high efficiency GaInP₂/GaAs system will focus on determining passivating conditions to further reduce or even eliminate corrosion. Further experiments are planned to look at surface pretreatments to see if NREL can increase the lifetime of the catalytic coat. NREL is also studying the influence of metallated and unmetallated porphyrins and phthalocyanins.

Task 2: Low Cost Amorphous Silicon Multijunctions

For this work NREL is partnering with Energy Conversion Devices (ECT) to grow samples specifically for water splitting. For these samples, two areas of research are of interest: 1) a device structure that pushes electrons toward the semiconductor/electrolyte interface and 2) protective coatings for the surface that offer minimum light absorption, but stability at high and low pH. The reason NREL and ECT want electrons to be driven toward the semiconductor electrolyte interface is because they want hydrogen to be evolved from the illuminated surface. Of the two reactions involved in water splitting (hydrogen evolution and oxygen evolution), hydrogen evolution is the easiest, requiring the least amount of catalyst and it has the lowest overvoltage. They also expect that it will be easier to protect a surface under reducing conditions than under oxidizing conditions.

Among the coating of interest are a-SiC, ITO, and SnO:F. Preliminary work at NREL has shown that a-SiC can provide a stable surface layer and is effective at protecting the underlying photovoltaic layers. ITO is also a strong possibility due to its use as a transparent electrode. SnO:F is very stable, but it requires a fairly high substrate temperature for deposition. These higher temperatures can lead to major degradation in a-Si devices.

Photoelectrochemical Based Direct Conversion for Hydrogen Production National Renewable Energy Laboratory

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
High Efficiency Tandem Cell and New Material Characterization						
Characterization of nitride materials for stability and water splitting y, and organometallic surface modification techniques for band edge modification and control				◆		
Low Cost Amorphous Silicon Multijunctions						
Determination of stability and efficiency characteristics for a-Si structures					★	

FY 2001 Begins October 1, 2000

Photoelectrochemical Hydrogen Production – University of Hawaii

Photoelectrochemical (PEC) production of hydrogen from water using sunlight as the energy source is one of the most promising technologies for low-cost renewable hydrogen production. The approach at the University of Hawaii has been to use component and reactor modeling to identify high efficiency potentially low cost materials and system designs. Promising materials are then evaluated through extensive materials synthesis and characterization and finally by fabricating and testing photoelectrodes. Past achievements have included the demonstration of direct solar-to-hydrogen conversion efficiencies exceeding 7.8% using photocathodes fabricated from multijunction amorphous silicon solar cells (10% net electrical efficiency). These photocathodes were fabricated using high efficiency sputter-deposited thin-film electrocatalysts developed at UH and were configured with a separated anode in a small-scale hydrogen reactor.

While the initial demonstrations of high efficiency used separated anodes, the recent effort has focused on the development of photoelectrodes with fully integrated cathodes/anodes. This past year, we proposed a new design for a fully-integrated photoelectrode, one which could be fabricated entirely with thin film processing techniques compatible with large area manufacture. Based on earlier conceptual system designs, these integrated structures are fabricated on metal substrates. The process sequence to fabricate prototypes of the new photoelectrode has been demonstrated using monolithic stacked triple-junction a-Si cells supplied by the University of Toledo. The electrocatalysts, contact layers, and protective films required for this design was developed at UH.

The new integrated design, first described at the Hydrogen Program Review in May 2000, allows the use of planar series-connected solar cells (as opposed to stacked cells) which opened the door for very high efficiency thin film materials such as copper-indium-gallium-diselenide/cadmium-sulfide cells (19.1% record electrical efficiency). A multisource evaporation system for deposition system of CIGS films was set up and tested as part of the effort to increase photoelectrode efficiency. Optimization of the catalyst as well as the transparent-conductor and transparent-protective films is continuing with current work focused on eliminating pinholes, cracks and edge effects.

The primary objectives for FY2001 are to demonstrate the ability to fabricate integrated photoelectrodes which are stable in KOH electrolyte. These experiments will be conducted using the monolithic stacked multijunction amorphous silicon. Concurrently, experiments will be carried out to develop a fabrication process for series connected high efficiency CIGS photoelectrodes.

Task 1: Materials Research

The stability of CIGS films in KOH will be investigated including corrosion rates for films with differing composition and morphology. Process conditions for optimized protective films (e.g. ITO, TiO₂) and electrocatalysts (e.g. NiFeOx and CoMo) will be reported. Alternative materials as improved coatings and catalysts will be explored.

Task 2: Engineering Modeling and Analysis

This task includes integration of the electrical and electrochemical models developed under prior agreements with state-of-the-art optical models. The integrated model will be used to develop a quantitative comparison of the stacked a-Si:H and lateral CIGS designs and for photoelectrode optimization.

Task 3: Photoelectrode Development and Testing

Photoelectrodes will be fabricated and tested to determine the performance characteristics of new materials and new designs under real operating conditions. Operation of an integrated photoelectrode for a period of at least 100 hours in KOH is the critical milestone, requiring a full processing sequence and pinhole free protective films. Preliminary component testing for CIGS-based photoelectrodes will also be conducted using our test photoreactor designed for 1" x 1" photoelectrodes.

Photoelectrochemical Hydrogen Productions University of Hawaii						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Materials Research						
Complete literature survey		◆				
Select catalyst and protective films for a SiH photoelectrode			◆			
Complete testing of CIS/CIGS materials			◆			
Report process conditions for optimal CIGS				◆		
Engineering Modeling and Analysis						
Complete integration of optical and electrical models			◆			
Analyze a Si:H photoelectrode performance			◆			
Analyze a CIGS photoelectrode performance				◆		
Report comparison of a Si:H and CIGS photoelectrodes					★	
Photoelectrode Development and Testing						
Test a Si:H integrated photoelectrodes		◆				
Test CIGS photoelectrode test structures			◆			
Report results of 100 hr stability test (a Si:H photoelectrodes)					★	
Report recommendations for optimal photoelectrode systems						★
FY 2001 Begins October 1, 2000						

PHOTOBIOLOGICAL PROCESSES

Development of an Efficient Algal H₂-Producing System – National Renewable Energy Laboratory

The concept of this project is to apply classical and molecular genetic techniques in order to engineer a green alga capable of sustained photobiological H₂ production at high rates in air for use in a direct water-splitting process that can be commercialized for renewable fuel production. The goals and objectives are to generate O₂-tolerant, high H₂-producing mutants from the green alga *Chlamydomonas reinhardtii*, test them in a laboratory-scale system for continuous photoproduction of H₂ under aerobic conditions, and collaborate with other national laboratories and universities in improving the efficiency of algal H₂ production.

Hydrogen production by green algae has significant advantages over other biological systems: ATP production is not required, high theoretical efficiencies are possible, and water is used directly as the source of reductant without the need to store intermediary carbon metabolites. Currently, the main practical biological limitations to using green algae for photobiological H₂-production are the sensitivity of the reversible hydrogenase to O₂ and low algal photosynthetic conversion efficiencies at solar light intensities. NREL will address the former problem, by generating and selecting for O₂-tolerant, H₂-producing mutants of *C. reinhardtii* using molecular genetic approaches.

There is sufficient precedent in the literature to warrant attempts to generate an O₂-tolerant hydrogenase in *C. reinhardtii* at this time. For example, O₂-tolerant hydrogenases have been reported in non-photosynthetic bacteria, photosynthetic bacteria, and *C. reinhardtii* mutants (although mutants in the latter organism were not preserved for future studies). Also, studies involving site-directed mutagenesis of the uptake hydrogenase from the bacterium *Azotobacter vinelandii* indicate that a single amino acid change in the sequence of one of the subunits of the enzyme alters the O₂-tolerance of the enzyme. Two generations of mutants were identified using classical mutagenesis techniques that have shown up to a factor of 10 increase in O₂ tolerance. These promising mutants will serve as the basis for NREL's continued activities. With these successes, NREL is ready to move forward with an aggressive molecular biology approach. They have obtained a clone of the reversible hydrogenase gene in *C. reinhardtii* that covers most of its active site for use in applying more powerful molecular biological techniques to improve algal O₂ tolerance. Their classical genetic approach has involved mutagenesis and selection under both photoreducing conditions (which favor O₂-tolerant, H₂-uptake activity of the enzyme), and H₂-producing conditions (which favor O₂-tolerant, H₂-evolving activity of the hydrogenase).

Task 1: Close out of the Classical Genetics Approach

The application of two selective pressures, based either on the H₂-producing or on the H₂-uptake activity of the reversible hydrogenase, have been combined in the past with the application of a chemochromic screening technique to isolate H₂-producing mutants of *C. reinhardtii* with increased tolerance to O₂. Two generations of mutants with a higher O₂ I₅₀ (estimated from the initial rates of light-induced hydrogen evolution measured amperometrically and by gas chromatography) were isolated. Current attempts to isolate a new generation of improved mutants using similar techniques have been unsuccessful, possibly indicating limitations of the mutagenesis/selection approach. Thus NREL is closing out the classical approach to generate new mutants, but will attempt to improve the phenotype of their current mutants (see Task 3). The last activity on this task will be the submission of a peer-reviewed paper reporting the current results.

Task 2: Molecular Biological Approach

With the development of new molecular biological tools, this approach to producing better O₂-tolerant mutants is very promising. NREL has currently cloned and sequenced the active site (about 2/3 of the algal hydrogenase gene). In order to complete the cloning they will examine two approaches: (a) use of RT-PCR to amplify mRNA from induced cells using degenerate primers specific for the active site of other Fe-only hydrogenases; and (b) sequence of clones from a cDNA library that hybridize to their partially cloned hydrogenase sequence. The identity of the gene will be confirmed by analysis of its sequence (for example by comparison with the sequence of other known hydrogenases) and by heterologous expression of the gene in *E. coli*. Simultaneously, NREL is chemochromically screening an insertional mutagenesis library (obtained from Prof. Melis, UC Berkeley) for clones that cannot produce hydrogen due to interruption of the hydrogenase gene. These clones will be useful in future studies as background strains for transformation with *in vitro*-mutated hydrogenases. These mutants will be obtained by directed evolution (random mutagenesis of the cloned gene) and/or site-directed mutagenesis.

Task 3: Identification of the Molecular Nature and Genomic Location of NRELs Current O₂-tolerant Mutations

Even though the classical genetics approach for generation of improved O₂-tolerant algal mutants is being discontinued, NREL will still attempt to improve the phenotype of their current mutants by performing genetic crosses between them. This will succeed, however, only if the different mutations involve different genes (loci). In order to accomplish this analysis, they will: (a) genetically cross four of their best current mutants with each other and screen the resulting progeny for mutants with higher O₂ tolerance; (b) map the locus (or loci) responsible for the O₂-tolerant phenotype in each of their four best mutants to identify the genes involved. This last step will be done in collaboration with L. Mets, University of Chicago, who has extensive expertise in *Chlamydomonas* genetics and has identified a number of well-defined markers on this alga's genome. If any of the mutations are on the hydrogenase gene, the mutated gene will be sequenced and compared to that of the wild-type strain to identify regions of the protein that may confer higher O₂ tolerance to its activity in support of Task 2.

Development of an Efficient Algal H₂-Producing System National Renewable Energy Laboratory

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Close out of the Classical Genetics Approach						
Submission of peer-reviewed paper to an appropriate journal.		◆				
Molecular Biological Approach						
Complete the screening of a cDNA library for clones that hybridize to NRELs partial sequence of the algal reversible hydrogenase				★		
Identification of the Molecular Nature and Genomic Location of NRELs Current O₂-tolerant Mutations						
Develop techniques to successfully perform genetic crosses and to screen the resulting progeny.					◆	

FY 2001 October 1, 2000

Hydrogen Production by Photosynthetic Water Splitting - Oak Ridge National Laboratory

Three key or advances in Fiscal Year 2000 that contribute to the goals of DOE's Hydrogen Program are reported. First, ORNL reported the discovery of a new oxygen-sensitive pathway and its role in photosynthetic hydrogen evolution. ORNLs data point to a hitherto unknown competitive pathway between hydrogen production and oxygen reduction. Previous thinking in this field attributed oxygen sensitivity of algal H₂ production to the inhibitory effect of O₂ on hydrogenase per se. However, a new role for oxygen in *Chlamydomonas reinhardtii* was observed that is clearly distinct from the oxygen sensitivity of hydrogenase. This pathway, with O₂ acting as electron acceptor, drains electrons away from the hydrogenase-catalyzed H₂ production pathway to O₂, thereby lowering the output of hydrogen. This pathway is more sensitive to O₂ than the oxygen sensitivity of hydrogenase. ORNL has obtained conclusive evidence that this pathway operates at an O₂ level as low as 1000 ppm which is well below the level of O₂ that inhibits hydrogenase activity. Their data further demonstrated that the newly discovered pathway requires the formation of proton gradients to function. This alternative pathway can be shut off by addition of 5 micromolar FCCP (a proton uncoupler), resulting in improved photoproduction of H₂. Second, they report the first measurements of sustained simultaneous photoevolution of hydrogen and oxygen in a confined photobiological reactor. This new concept in reactor design takes advantage of the Henry's Law equilibration between liquid and gas phases for hydrogen and oxygen that is photoproduced in the liquid phase. Third, ORNL has completed their initial experiments on improvement in photosynthetic activity in mutants of *Chlamydomonas reinhardtii* that genetically reduced antennal sizes. A manuscript on this work has been submitted for publication in a peer-reviewed scientific journal. In addition to this work, they continue their enthusiastic collaboration with Drs. Michael Seibert and Maria Ghirardi at the National Renewable Energy Laboratory and with Prof. A. Melis at the University of California, Berkeley.

Task 1: Role of a New Pathway in Maximizing Hydrogen Production by Photosynthetic Water Splitting

As described above, ORNL report the discovery of a new oxygen-sensitive pathway and its role in photosynthetic hydrogen evolution. Their data point to a hitherto unknown competitive pathway between hydrogen production and oxygen reduction. This pathway is more sensitive to O₂ than the hydrogenase and requires a proton gradient to operate. This discovery forms the basis for a rational approach to understanding the nature of background oxygen and its inhibitory effect on photosynthetic hydrogen production. The focus of this task is on understanding the new pathway associated with the presence of oxygen. The data suggest that eliminating this electron drain pathway in the presence of oxygen can have a significant impact on photosynthetically produced hydrogen and oxygen.

Task 2: Photobiological Reactor Engineering Design

Another key goal of this project is the development of photobiological reactors for hydrogen and oxygen production. ORNL has had initial success by performing the first experiments in which hydrogen and oxygen were simultaneously evolved in a confined reactor. The goal of this task is to extend these promising results which are now being written-up for publication in a peer reviewed scientific journal. Specifically, the new experiments of this task will focus on the effect of dwell time on hydrogen and oxygen productivity. Additional experiments on the relationship between headspace and liquid volume will also be performed. The goal of this project is clear: to use the best algal mutants in the most efficient photobiological reactor for optimizing the yields of hydrogen and oxygen production. This task will be performed in collaboration with Prof. L. Mets of the University of Chicago.

Task 3: Linearization of the Light-Saturation Curve of Photosynthesis

In addition to efficient simultaneous photoproduction of hydrogen and oxygen, linearization of the light-saturation curves is a key scientific challenge for the field of renewable hydrogen production by photosynthetic water splitting. Since photosynthesis saturates with increasing light intensity, a loss of efficiency and potential productivity occur at higher solar irradiances. ORNL has had initial success in working with a mutant of *Chlamydomonas reinhardtii*, that had an antennal size approximately 1/4 that of wild-type. This task will continue these promising results by further shrinking the antenna size. From a practical and economic point of view, the ultimate goal is to develop an algal system that has a completely linear light saturation curve for all values of terrestrial solar irradiation.

Hydrogen Production by Photosynthetic Water Splitting Oak Ridge National Laboratory

Task Designation/Milestone	2001					2001
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
New Pathway						
Effect of ionophores			◆			
Complete manuscript				◆		
Reactor Design						
Effect of dwell time					◆	
Linearization Studies						
Complete manuscript				★		
Further antenna reduction						◆

FY 2001 Begins October 1, 2000

Maximize Photosynthetic Efficiencies and Hydrogen Production in Microalgal Cultures - University of California, Berkeley

The goal of this research is to produce genetically engineered microalgae with enhanced photosynthetic solar conversion efficiencies and hydrogen production under mass culture conditions. To achieve this, it is necessary to minimize the light-absorption capability of the photosystems, a solution that requires reduction in the number of the chlorophyll molecules that service the two photosystems. This will be achieved through DNA insertional mutagenesis and screening of the model green alga *Chlamydomonas reinhardtii*, and via biochemical, genetic and molecular analyses of the transformant cells. The goal is to clone the gene(s) that cause a “truncated chlorophyll antenna size” in photosynthesis. A truncated light-harvesting chlorophyll antenna size for photosystem-II and photosystem-I will result in a relatively higher light intensity for the saturation of photosynthesis in individual cells. However, it will permit an overall greater solar energy conversion efficiency and cellular productivity in dense cultures because it will minimize wasteful absorption and dissipation of bright incident sunlight. A truncated chlorophyll antenna size will moreover alleviate mutual cell shading and photoinhibition in the mass culture. A recently completed feasibility study has shown that, in mass culture, algal strains with a transiently truncated chlorophyll antenna size exhibited ~3 times greater rates of photosynthetic productivity than could be achieved with fully pigmented cells. The proposed research seeks to develop green algal strains having a permanently truncated chlorophyll antenna size, and to isolate and characterize the genes and proteins that regulate the chlorophyll antenna size of photosynthesis. This information will find direct application in photobiological hydrogen production.

Recent work focused on the biochemical analysis of a Chl *b*-less mutant of *Chlamydomonas reinhardtii*. Through DNA insertional mutagenesis the University of California at Berkeley also isolated a regulatory mutant with a truncated light-harvesting chlorophyll antenna (termed *tlh1* on the basis of the presumed gene that has been interrupted by the DNA insertion). Biochemical, genetic and molecular analyses of the *tlh1* transformant will be the priority of work in FY 2001. At the same time, further DNA insertional mutagenesis will be applied for the generation and isolation of additional transformants with a ‘truncated chlorophyll antenna size’. The isolation of more than one *tlh* mutants will ensure that more than one genes responsible for the down-regulation of the chlorophyll antenna size in photosynthesis have been “hit” and that, in the end, all such regulatory genes have been identified.

Task 1: DNA Insertional Mutagenesis Library

Expand the library of *Chlamydomonas reinhardtii* DNA insertional transformants from the current 6,500 to 12,000 total in order to isolated additional transformants with a ‘truncated chlorophyll antenna size’.

Task 2: Cryopreservation

Continue with the development and testing of the cryopreservation method that will permit an indefinite storage of the above library. This library will be a significant resource for the DOE H₂ program.

Task 3: Solar Conversion Efficiency and Productivity Measurements

Characterize the structural-functional organization and provide a measure of the solar conversion efficiency of the photosynthetic apparatus in selected *Chlamydomonas reinhardtii* transformants, which have a significantly truncated chlorophyll antenna size.

Task 4: Genetic Analysis of Truncated Chlorophyll Antenna Mutants

Genetic crosses of the selected transformants will test for co-segregation of the "truncated antenna" and "arg+" phenotypes in the mutants. Linkage of the "truncated antenna" property to the arg+ gene insertion will be tested by analysis of the progeny from the back-cross of the putative "truncated antenna" strains with the arg-2 auxotrophs. Mutants will be selected on the basis of co-segregation of the "truncated antenna" and "arg+" phenotypes. This co-segregation is an important prerequisite for the subsequent cloning of the gene interrupted by the exogenous DNA insertion because it signals the presence of the "tag" in the position of the lesion. Identification, cloning and sequencing of the gene(s) responsible for the down-regulation of the Chl antenna size in *Chlamydomonas reinhardtii* will open the way for direct manipulation of the Chl antenna size in many other algae and higher plants of interest to the DOE Hydrogen Program.

Task 5: Southern (Genomic) Blot Analysis of Transformants

Genomic DNA of cells transformed with the cloned DNA will be subjected to Southern blot analysis with a probe specific for the ARG7 gene and, separately, with the cloning vector. This comparative Southern blot analysis will provide a way to visualize the number of independent insertions of plasmid/ARG7 genes in the *C. reinhardtii* genome and it will complement the genetic analysis outlined in (D) above.

Task 6: Initiate Gene Cloning

The Southern (genomic) blot analysis of the transformants and the restriction maps that will thus be generated will form the basis of efforts to clone the genomic DNA that is flanking the insertion. Following the construction of the respective restriction maps, efforts at cloning of the disrupted gene will be initiated.

Task 7: Preparation of Reports on the Results

Maximizing Photosynthetic Efficiencies and Hydrogen Production in Microalgal Cultures University of California, Berkeley						
Task Designation/Milestone	2001					2001
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Expand DNA insertional mutagenesis library, screen for truncated Chl antenna size (<i>tlh</i>) mutants		◆				
Cryopreservation of the DNA insertional library		◆				
Provide solar conversion efficiency measurements for the new <i>tlh</i> mutants			◆			
Perform genetic analysis of the <i>tlh</i> mutants			◆			
Perform southern (genomic) blot analysis of the <i>tlh</i> mutants and construction of restriction mapping in the vicinity of the insertion			◆			
Initiate efforts at gene cloning				◆		
Identify a group of mutants with significantly truncated Chl antenna size, suitable for the goals of the program in which to identify target genes					★	
Prepare reports	◆					◆
FY 2001 Begins October 1, 2000						

A Cyclic Photobiological Algal Hydrogen Production System – National Renewable Energy Laboratory

The concept of the project is to fully develop and optimize an innovative photobiological H₂ production system based on the down-regulation of photosynthetic O₂ evolution in the green alga *Chlamydomonas reinhardtii* by temporarily depleting the growth medium of sulfur. The resulting H₂ production activity of the culture will be a prelude to a viable commercial H₂-production system. The objective of the effort is to metabolically regulate photosynthetic O₂ evolution, allowing algal cultures to go anaerobic by physiological means, induce the hydrogenase enzyme and evolve large amounts of H₂; to reversibly shift the culture between aerobic O₂ evolution and anaerobic H₂ production modes to prolong the H₂ production activity.

Previous algal H₂-production systems utilized O₂-scavenging components (such as sodium dithionite or the glucose/catalase/glucose oxidase mix) or neutral gas purging to constantly remove photosynthetically generated O₂ from the algal culture growth medium. These methods allowed the culture to produce H₂ on a continuous basis, but they are not cost effective. NREL's current algal system does not need external O₂ scavenging, produces H₂ in the light for up to 3 days, and can be recycled at least 3 times between normal photosynthetic and H₂-producing modes.

Recent biochemical evidence strongly indicates that the reductants necessary for photobiological H₂ production originate mainly from the residual photosynthetic activity of sulfur-depleted cells. Furthermore, some H₂ production may also result from substantial internal protein degradation. Current rates of H₂ production are about 25% of the maximum rates of residual photosynthetic H₂O oxidation, suggesting that up to only one fourth of the electrons generated from H₂O are being utilized for H₂ production. Nevertheless, current rates of H₂ production are comparable to the rates of H₂ production by systems in which 100% of the H₂O oxidation activity is present, and which utilize non-physiological means to scavenge O₂ from the medium.

Initial research efforts will focus on the investigation of conditions that may result in even faster, specific, and reversible inactivation of photosystem II O₂ evolution activity, and on improvements in the yield of H₂ production exhibited by the current system. More specifically, NREL will investigate whether additional physiological manipulations by themselves or in combination with their current procedures will accelerate the process of photosystem II inactivation, and whether exposure to additional stress conditions may similarly affect this process. In order to improve the yields of the current system, experiments will be designed, initially, to address the following two tasks: (1) determine the rate-limiting step controlling current H₂-production activity and (2) optimize the H₂-production process. Other studies will also continue to investigate the biochemical pathways involved in H₂ production under sulfur-depleted conditions.

Task 1: Determine the Rate-Limiting Step Controlling Current H₂-Production Activity

This task will address the following possibilities in detail: (a) build-up of H₂ during the H₂-production phase, which, due to the reversible nature of the enzyme, limits the rate of the forward H₂-releasing reaction (in collaboration with ORNL); (b) competition for reductant between the normal photosynthetic CO₂-fixing system and the hydrogenase pathway, leading to lower rates of H₂ evolution; (c) limitations in the rate of mobilization of stored metabolites, transport of reductant to the photosynthetic apparatus (photosystem I), or hydrogenase enzyme levels; and (d) reductant generation by residual hydrogen oxidation activity.

Task 2: Optimize Process

This task will examine such parameters as: (a) treating the cultures under additional stress conditions to more rapidly inactivate photosystem II activity; (b) altering the physiological conditions that lead to inactivation of O₂ evolution to speed up the switchover to anaerobic conditions; (c) finding ways to eliminate the requirement for acetate during inactivation of O₂ evolution; (d) examining the loss of collected H₂ gas due to a less than optimal gas collection design and (e) testing NREL's current O₂-tolerant mutants' performance in this H₂-producing system. NREL will utilize their automated system in order to speed up the process.

Once the rate-limiting step in H₂ production by the system is determined, appropriate measures will be taken to alleviate it. For example, if it is found that the rates of H₂ evolution are inhibited by competition with the CO₂ fixation pathway, NREL will attempt to find mutants that have a less efficient Rubisco (the enzyme that is responsible to committing electrons from photosynthesis to CO₂ fixation).

The ultimate goal of this work is to develop a mid-term hydrogenase-based, H₂-production system that can lead to a viable commercial process before an O₂-tolerant hydrogenase system can be developed.

A Cyclic Photobiological Algal Hydrogen Production System National Renewable Energy Laboratory

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Determine the Rate-Limiting Step Controlling Current H₂-Production Activity						
Complete the study of the effect of different metabolic inhibitors on the H ₂ production rates by sulfur-depleted cultures.				◆		
Optimize Process						
Complete investigation of other conditions that might accelerate the process of O ₂ evolution inactivation and the switching over to anaerobic conditions. September 2000					★	

FY 2001 Begins October 1, 2000

Efficient Hydrogen Production Using Enzymes Of The Pentose Phosphate Cycle – Oak Ridge National Laboratory

Research has focused on the optimization of a novel *in vitro* enzymatic H₂ production system that employs (mesophilic) enzymes composing the oxidative branch of the pentose phosphate cycle. In addition, work is being carried out to isolate and clone the genes for the hyperthermophilic counterparts of these enzymes from *Sulfolobus solfataricus*. To increase the production of hydrogen from biomass-derived glucose and achieve the maximum molar yield of by employing the enzymes of the pentose phosphate cycle in conjunction with the hydrogenase from *Pyrococcus furiosus*. This process centers on three NADP dependent enzymes, glucose-6 phosphate dehydrogenase (G-6-PDH), 6-phosphogluconate dehydrogenase (6-PGDH) and hydrogenase from *Pyrococcus furiosus*. The dehydrogenases are currently obtained from mesophilic sources. However, in order to increase the rates of hydrogen production, work is being carried out to isolate the genes for the glucose-6 phosphate dehydrogenase, and 6-phosphogluconate dehydrogenase from *Sulfolobus solfataricus*. This involves the production of *Sulfolobus solfataricus* genomic DNA and the following techniques, PCR, Southern blotting and hybridization. The final aim is to eventually express these recombinant enzymes in a mesophilic host such as *Escherichia coli* and incorporate them into an entirely hyperthermophilic *in vitro* enzymatic H₂ production system.

Task 1: Determination of The Rate-Limiting Steps that Regulate the Oxidative Pathway of the Pentose Phosphate Cycle For Maximum H₂ Evolution.

Task 2: Generation of Recombinant Form of 6-Phosphogluconate Dehydrogenase from *Sulfolobus solfataricus*.

Task 3: Identify the Gene for Glucose-6-Phosphate Dehydrogenase from *Sulfolobus solfataricus*.

Task 4: Cloning, Expression, and Characterization of Recombinant 6-Phosphogluconate Dehydrogenase.

Efficient Hydrogen Production Using Enzymes of the Pentose Phosphate Cycle Oak Ridge National Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Determination of the rate-limiting steps that regulate the oxidative pathway of the pentose phosphate cycle for maximum H ₂ evolution	◆					
Generation of recombinant form of 6-phosphogluconate dehydrogenase from <i>Sulfolobus solfataricus</i>			◆			
Identify the gene for glucose-6-phosphate dehydrogenase from <i>Sulfolobus solfataricus</i>				◆		
Cloning, expression, and characterization of recombinant 6-phosphogluconate dehydrogenase					◆	
Clone, express, and characterize recombinant glucose-6-phosphate dehydrogenase from <i>Sulfolobus solfataricus</i>					◆	
Optimization of the oxidative portion of the pentose phosphate cycle using extremely thermophilic forms of glucose-6-phosphogluconate dehydrogenases						★

FY 2001 Begins October 1, 2000

Task 5: Clone, Express, and Characterize Recombinant Glucose-6-Phosphate Dehydrogenase from *Sulfolobus solfataricus*.

Task 6: Optimization of the Oxidative Portion of the Pentose Phosphate Cycle Using Extremely Thermophilic forms of Glucose-6-Phosphate and 6-Phosphogluconate Dehydrogenases.

International Energy Agency and Other International Collaborations – National Renewable Energy Laboratory

The objective of this project is to foster international collaborations and technology transfer for the advancement of hydrogen production, storage and utilization technologies. Included is support for activities conducted within the framework of the International Energy Agency (IEA). NREL provides the Secretariat function, as well as the Task Leader for the Integrated System activities and experts for the Photoelectrochemical Hydrogen Production, Carbon for Hydrogen Storage, Hydrogen Production from Carbon Containing Materials and Integrated Systems tasks, all for the IEA Hydrogen Agreement and provides an expert on biomass pyrolysis and pyrolysis oils for the IEA Bioenergy Agreement. This project also provides support for an international collaboration to develop steam reforming of bio-oil with the University Rovira i Virgili, Spain.

Task 1: Secretariat Support

NREL is responsible for the day-to-day operations of the IEA Agreement on the Production and Utilization of Hydrogen and serves as the administrative arm of the Executive Committee. This includes organizing and reporting on the Executive Committee meetings, producing the Annual Report, managing the Common Fund, monitoring the progress of all Annex activities, and reporting to IEA Headquarters, as well as coordinating various strategic planning activities.

Task 2: Integrated Systems Operations (IEA Hydrogen Agreement Annex 13)

The objective of Annex 13, Design and Optimization of Integrated Systems, is to develop a tool to assist in the design and evaluation of potential hydrogen demonstration projects and in the optimization of existing hydrogen demonstration projects. Emphasis will be placed on integrated systems covering all components, from input energy to end use. The activities will be focused on near- and middle-term applications, with consideration of the transition to sustainable hydrogen energy systems. Component models developed under a previous task will be updated and refined to include cost information. Finally, life cycle assessments will be performed on comparative hydrogen systems.

NREL serves as the Operating Agent (OA) for Annex 13. In this capacity, overall organization and technical and administrative management of the activity are required. In addition, the OA is required to report on a regular basis to the Executive Committee, and to provide detailed reports as stipulated in the Annex 13 work plan.

Task 3: International Collaborations

Participation in IEA Hydrogen Agreement Integrated Systems Activities: Existing and proposed hydrogen energy system demonstrations typically deploy technologies at different levels of development. A combination of data collection, demonstration case studies, component simulation, integrated systems modeling and life cycle assessment will result in the development of design guidelines for future demonstrations.

NREL expertise in life cycle analysis and process simulation and analysis are critical to the success of this activity. Participation is required in Subtask A (Model Development) and Subtask B (Systems Analysis) of Annex 13.

Participation in IEA Collaborative on the Study of the Amorphous Silicon Carbide/Electrolyte Interface and other Novel Water Splitting Systems (Hydrogen Agreement Annex 14, Photoelectrolytic Production of Hydrogen): The aim of this task is to develop a stable semiconductor/electrolyte based water splitting system. This will be a joint effort involving researchers from the University of Geneva and the University of Berne in Switzerland, Uppsala University in Sweden, and the National Renewable Energy Laboratory. This cooperative research program will use the strength and capabilities of each member of the research team.

This research will involve the growing and characterization of various compositions and structures of thin films. NREL will do solid state and material characterization including SIMS, XPS and Auger, and study the semiconductor/electrolyte interface using impedance spectroscopy. The University of Geneva will study the fundamental photoelectrochemical properties, including photocurrent voltage measurements and spectral response. The goal of this research is to determine the best composition and growth parameters that give rise to the most stable interface while maintaining high conductivity and optical transparency, as well as studying some new structures for possible application as water splitting devices.

With the University of Geneva, Switzerland, NREL will be investigating some novel configurations involving a unique tungsten trioxide (WO_3) electrode that they have developed. These electrodes will only split water with a 0.6 v external bias. NREL proposes to provide this bias with an amorphous silicon tandem cell from ECD. The configuration would be a standard WO_3 electrode on glass with an a-Si cell directly behind it. This could be a very inexpensive water splitting setup, since they could use the standard commercial a-Si cells, and they would never be in contact with the electrolyte. Also the WO_3 is infinitely stable in water. As part of this collaboration, Ms. Clara Santos from the University of Geneva visited NREL for two months in the summer of 1999 to perform some experiments. NREL determined the band edge positions for a few WO_3 samples. As expected, the material is n-type, but there is some variability in the measured band edge position. This is important as it determines the nature of the a-Si cell NREL will use to make the tandem device. Ms. Santos is finishing her PhD, and is applying for a Swiss scholarship for a postdoctoral position at NREL. NREL will continue this work should she receive this scholarship.

Uppsala University (Sweden) has developed synthetic procedures for "purpose built materials;" that is, the controlled assembly of Fe_2O_3 , ZnO and Ru oxides in the nanoparticle regime into various shapes. Moreover, these samples can be prepared on flexible substrates. Their initial investigations of this new Fe_2O_3 material showed that it has higher quantum yields than the regular material, but has a low efficiency due to the thin film not absorbing much light. Stability is also an issue. NREL is continuing to evaluate this material for water splitting. This will involve some changes in the synthesis, and some adjustments in the experimental procedures.

A new project has been initiated with Professor Gion Calzaferri at the University of Berne, Switzerland. He has a catalytic system that uses a silver-based photo-electrode to produce oxygen under illumination. Since GaInP_2 will produce hydrogen (but not oxygen), NREL has given him some GaInP_2 electrodes to try in his system to see if a tandem configuration will be able to split water.

Two projects are in the discussion stages with countries that are considering joining the Annex (and the IEA Hydrogen Agreement). One of the projects involves Australia (and possibly New Zealand), and would be aimed at developing an integrated amorphous silicon system for water splitting. The second project involves Mexico and would focus on thin film systems based on copper-gallium-indium diselenide systems. Dr. Arturo Fernandez from UNAM, Mexico is spending his sabbatical year at NREL, and NREL will work to develop a joint collaborative project during that time.

Photobiological Production of Hydrogen: Biological hydrogen production, the production of H₂ by microorganisms, has been an active field of basic and applied research for over two decades, with significant applied R&D programs supported in Europe, Japan and the USA. The IEA Hydrogen Agreement has had active tasks focusing on this subject for six years now, starting with the recently completed Annex 10, Photoproduction of Hydrogen, and now with the new Annex 15, Photobiological Production of Hydrogen. The recent advances in producing measurable quantities of hydrogen using green algae is of significant importance to the success of this international collaboration. NREL significant expertise in this area will be essential to the success of this task.

This year NREL researchers will collaborate with international representatives from the University of Uppsala, Sweden, the Norwegian Institute for Water Research, the University of Montreal, Canada, and the University of California to further the fundamental understanding of the genetics, biochemistry and physiology of hydrogenase functions, including the metabolism and factors affecting growth of microalgae.

Participation in IEA Pyrolysis Activity: The IEA Bioenergy Pyrolysis Activity (PyRA) merged in 1998 with the European Community sponsored network PyNE. The new network (PyNE) includes eighteen members: the U.S., Canada, Brazil, and fifteen European countries. During FY2000 PyNE completed its term of work and began developing the work scope for the next phase. The overall objective of the new term will be to improve the rate of implementation of fast pyrolysis technologies for the production of fuels and chemicals. Key to this objective will be to reach resolution on some of the critical technical areas that were part of the earlier phase of work. Dissemination of relevant information to industry and to policy makers will also be an important component of the effort. Much of the PyNE emphasis will be placed on the production of bio-oil for power and heat applications. As during the previous phase of work, the network activities will be organized in subject groups: Market Development for Fast Pyrolysis and Bio-oil; Fuel Standards for Bio-oils; Environment, Health, and Safety; New Technologies for Production of Bio-oils; and Applications of Bio-oils. A kick-off meeting will be held in early 2001 to finalize the activity structure and program of work. Dr. Stefan Czernik will continue as the U.S. representative to the network and as a member of the steering committee. He will also assume leadership of the Applications of Bio-oils Group. The overall objective of this group will be to review the existing applications of bio-oils and to explore future opportunities.

Collaboration with the University Rovira i Virgili (Spain): For the past four years, this collaborative effort has resulted in significant advances in the area of steam reforming bio-oil and hemicellulose-rich liquids from biomass fractionation processes to produce hydrogen. This year NREL will continue to investigate other biomass-derived liquids (vegetable oils and byproducts from bio-diesel processes) as feedstocks for the steam reforming process. This effort will be carried out through a researcher exchange program between NREL and the University Rovira i Virgili. In June 1998 the Commission for Cultural, Educational and Scientific Exchange awarded funding support for the U.S./Spanish collaborative project: "Hydrogen Production by Steam Reforming of Liquid Byproducts and Wastes Derived from Biomass Fractionation."

Collaboration for the Development of Carbon Nanotubes for Hydrogen Storage: IEA Task 12, Metal Hydrides and Carbon for Hydrogen Storage, will be concluded this year with the completion of the final report. Efforts will be focused on summarizing the single-wall nanotube project (two-year collaborative project with the University of Montpellier), as well as contributing to the development of the new IEA hydrogen storage task, Task 17. NREL will play a key role in defining the scope of the new task related to carbon materials for hydrogen storage.

In support of the continuing collaborations for hydrogen storage, NREL will work with Prof. Richard Chahine at l'Universite du Quebec a Trois_Rivieres. This activity will be included in the new IEA Task 17 and will be focused on obtaining adsorption isotherms on raw and purified single-wall carbon nanotube materials with different kinds of probe molecules (He, Ar, CH₄, H₂, etc). The purified materials may be supplied in either annealed or un_annealed forms that are expected to have different internal surface area properties. Initially, materials will not be supplied activated for hydrogen storage. These background experiments will yield information that will be relevant to understanding these materials for hydrogen storage applications. Activated samples will be subsequently supplied. This Task will facilitate international collaboration by providing for interchange of information between all IEA members collaborating within Task 12.

Support for the Project Development of a New IEA Activity on Hydrogen Production for Carbon Containing Materials: NREL's expertise in the area of biomass conversion and utilization will be essential during the planning phase for this new IEA project. Experts will participate in one or more international planning workshops to ensure that the collaborative activities are aligned with DOE Hydrogen Program objectives and that appropriate industry representatives are included. NREL will also have a key role in drafting the Programme of Work for this 3-5 year activity. Upon formalization of this task, Dr. Robert Evans of NREL will serve as the Subtask Leader for activities involving hydrogen production from biomass.

**International Energy Agency and Other International Collaborations
National Renewable Energy Laboratory**

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Secretariat Support						
ExCo Meetings		◆		◆		
2000 Annual Report					◆	
Integrated Systems Operations						
Conduct Expert Meetings	◆			◆		
International Collaborations						
LCA of Integrated Systems					★	

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3.1.2 Hydrogen Storage Research Projects

A key component of hydrogen R&D is the development of storage systems for hydrogen. Stationary storage systems are needed to provide hydrogen for electricity generation to complement distributed and intermittent renewable resources and to store off-peak energy for use during peak energy periods. Stationary storage systems will also be needed at vehicle refueling stations. Safe, lightweight hydrogen storage systems are needed for storing hydrogen on-board vehicles. Program hydrogen storage R&D is being conducted using carbon structures as well as metal hydride systems. Storage tasks are summarized in Table 3.3.

Table 3.3 Hydrogen Storage Research		
Goal: Demonstrate safe and cost-effective storage systems for use in stationary distributed electricity generation applications, and for on-board and stationary applications in non-attainment areas.		
Category	Project	Researcher
<i>Carbon Structures</i>	Feasibility of Fullerene Hydride as High Capacity Chemical Storage System	MER Corporation
	Carbon Nanotube Materials for Hydrogen Storage	National Renewable Energy Laboratory
	Doped Carbon Nanotubes for Hydrogen Storage	Westinghouse Savannah River Technology Center
<i>Metal Hydrides</i>	Catalytically Enhanced Hydrogen Storage	University of Hawaii
	Hydrogen Storage Development/Hydrogen Beds	Sandia National Laboratories
	Hydrogen Storage in Polymer-dispersed Metal Hydrides	United Technologies Research Center
<i>Physical Storage</i>	Vehicular Hydrogen Storage Using Lightweight Tanks	Lawrence Livermore National Laboratory
	Advanced Thermal Hydrogen Compression	Ergenics, Inc.

CARBON STRUCTURES

Feasibility of Fullerene Hydride as High Capacity Chemical Hydrogen Storage System - MER Corporation

Over the past several years MER has demonstrated the possibility of reversible hydrogenation of fullerenes and dehydrogenation of fullerene hydrides. Theoretically, fullerene molecule C_{60} can be hydrogenated up to $C_{60}H_{60}$, which corresponds to almost 7.7 wt.% hydrogen and, therefore, makes fullerenes attractive as a high capacity light weight hydrogen storage material.

Practically, the ability of fullerenes to store as much as 6.7 wt. % hydrogen was demonstrated, however, the dehydrogenation activity appeared to be slow due to the difficulty in breaking strong C-H bonds, which makes the overall hydrogen storage capacity lower than anticipated maximum potential.

MER has identified the key conditions required to maximize the reversible hydrogen storage in fullerenes, which include the following:

- Successful hydrogenation and dehydrogenation of fullerenes/ fullerene hydrides at mild conditions require a specific catalyst.
- Thermodynamically, equal amounts of hydrogen can be released easier from the compound with the higher initial hydrogen content.
- Since fullerenes are solid, presence of the liquid phase during the reaction is critical in order to provide better contact with catalyst
- Modification of the electronic structure of fullerenes is required to enhance hydrogenation and dehydrogenation by weakening C – H bonds.

During the course of this project MER will evaluate feasibility of using fullerenes as a high capacity, light weight and environmentally safe hydrogen storage material with the specific objectives including optimization of catalytically activated hydrogenation and dehydrogenation processes in order to maximize percentage of reversible hydrogen.

Task 1: Maximizing Hydrogen Content in Fullerene Hydride at Mild Conditions

While carrying out the first task, MER will optimize the usage of the selected liquid catalysts by establishing optimal loading, mixture preparation procedure and analyzing kinetics of the reaction at different temperatures and pressures. The modification of the electronic structure of fullerenes by doping with the electron donating intercalating elements will also be performed and its effect on hydrogenation with or without catalysts will be evaluated. At the completion of this task, the conditions will be established enabling maximum hydrogen content at moderate temperature and pressure.

Task 2: Optimize Dehydrogenation of Fullerene Hydrides

The critical part of the second task is facilitation of the dehydrogenation reaction, when the C – H bonds must be broken in order to release hydrogen. MER will evaluate the effect of the above techniques as well as temperature and initial level of hydrogenation on effectiveness of dehydrogenation to establish optimal conditions enabling lowest hydrogen content of the product. Repeatability of the results will be tested by cycling between hydrogenation and dehydrogenation at moderate temperature.

Feasibility of Fullerene Hydride as High Capacity Chemical Storage System
MER Corporation

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Maximizing Hydrogen Content in Fullerene Hydride at Mild Conditions						
Optimize catalyst usage			◆			
Modify electronic structure				◆		
Establish the temperature effect					◆	
Optimize Dehydrogenation of Fullerene Hydrides						
Evaluate the strength of C-H bonds at various hydrogen content				◆		
Facilitate the breakage of C-H bonds at moderate temperatures						★
Evaluate cycling ability						◆

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Carbon Nanotube Materials for Hydrogen Storage – National Renewable Energy Laboratory

Carbon single-wall nanotubes (SWNTs) consist of one cylindrical and closed graphite sheet without a seam and are therefore essentially elongated pores of nanometer dimensions. These carbon materials are unique in their ability to reversibly store and liberate hydrogen with small excursions in temperature and pressure about normal ambient values. This research program seeks to capitalize on the interaction between molecular hydrogen and these elongated pores to develop an adsorbent for hydrogen which will provide a safe, cost-effective, convenient, and energy efficient method for on-vehicle storage of hydrogen. Other non-SWNT carbon-based adsorption systems may also be investigated to evaluate their efficacy in comparison to the proposed SWNT system.

The goals and objectives of this project are to 1) produce large quantities of nanotubes with selected diameters, lengths, chiralities, and orientations in a cost-effective manner, 2) controllably access the sites which strongly and reversibly bind hydrogen so that 3) the kinetics, thermodynamics, and capacity of hydrogen adsorption may be simultaneously optimized. The long term goal is to scale-up production of optimized materials to enable ambient temperature and pressure adsorption of hydrogen at energy densities specified by the Hydrogen Program Plan (6.5 wt % and 65 kg/m³).

Numerous researchers have investigated activated carbon and other porous adsorbents for the storage of hydrogen and other gasses. For sufficiently small pores, the binding energy can be large enough to stabilize adsorbed hydrogen at room temperatures. Recently, NREL has found that charge-transfer effects can also lead to enhanced hydrogen adsorption properties. These types of effects may predominate in SWNT materials. Close-packed arrays of SWNTs offer a conceptually ideal adsorbent for hydrogen since all of the internal volume is of the nanoporous variety, and the material density is high. NREL demonstrated that hydrogen can be physically adsorbed on soots containing SWNTs with binding energies five times greater than is possible on planar graphite. They have recently developed methods to produce SWNT materials with a purity greater than 98 wt %, and demonstrated with these materials that hydrogen can be adsorbed in a density of at least 7 wt % from a room temperature, atmospheric-pressure ambient. Recent advances in the purity and rate of SWNT fabrication suggest that bulk and cost-effective production methods will soon be available. Thus, it is reasonable to work on developing a room temperature, room pressure hydrogen storage system based on SWNTs. The next phases of this work are focused on deepening the understanding of how these materials work, and developing their hydrogen storage capabilities at larger scales.

Task 1: Optimizing and Characterizing H₂ Uptake and Discharge

This year NREL plans to characterize the hydrogen adsorption on purified, cut SWNTs with their newly developed in-house Sievert's apparatus. NREL expects very good agreement between the volumetric and TPD methods. They will also collaborate with an outside laboratory to allow independent verification of their results. NREL also plans to study the effects of employing different metal hydrides such as Ti-Fe, Ti, Mg and Pd to assist the hydrogen adsorption process on SWNTs and to explore both different sonication and mechanical methods for incorporating the metal hydrides in the SWNT materials in an effort to up-scale their current adsorption activation process. Finally, they will further probe the charge transfer mechanism using in situ-Raman investigations in conjunction with conductivity measurements. A greater understanding of this process should enable maximum hydrogen storage capacities to be achieved.

NREL hopes to combine temperature-dependent Raman studies with infrared and uv-vis spectroscopies to achieve characterize the semi-conducting or metallic nature of individual SWNTs within nanotube samples. Developing such a method to characterize nanotube type will not only facilitate the development of SWNT-hydrogen storage technology, but will also constitute a very important contribution to the SWNT community at a basic science level.

Task 2: Nanotube Production, Purification, and Characterization

The new laser system will allow these aspects to be probed in more detail to enable high-yield and high-rate production of samples having specific types and diameters of tubes. The use of induction heating will also be explored to provide additional synthetic control and allow a higher throughput for SWNT production. These samples will be used in the hydrogen storage work described in Task 1, and be supplied to collaborators.

During this next year NREL will continue to investigate chemical vapor deposition (CVD) -based growth with a focus on (1) developing a detailed understanding of the fundamental mechanisms and (2) developing methods to scale-up the CVD production to produce multi-gram and perhaps kilogram quantities of SWNTs. The tubes contained in these CVD samples are inherently different in size, type, and quality than those produced by laser vaporization. The purification technique developed for laser-grown materials will be applied to the CVD materials and adapted as required. These samples will be used in the hydrogen storage work described in Task 1, and be supplied to collaborators. The behaviors and characteristics of the two different types of materials will be compared.

The synthesis work will require substantial characterization to assess the dimensions and quality of the SWNTs that will be produced. Raman spectroscopy, infrared spectroscopy, thermal gravimetric analysis, and transmission and atomic force microscopies will be used extensively.

Carbon Nanotube Materials for Hydrogen Storage National Renewable Energy Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Optimizing and Characterizing H₂ Uptake and Discharge						
Work with an independent laboratory to establish agreement between hydrogen uptake determinations made with temperature programmed desorption and those obtained with other techniques			◆			
Nanotube Production, Purification, and Characterization						
Produce gram-sized samples that consist of tubes of specific types. Correlate tube types with hydrogen adsorption properties.					★	

FY 2001 Begins October 1, 2000

Doped Carbon Nanotubes for Hydrogen Storage - Westinghouse Savannah River Technology Center

The ultimate goals of this project are to develop and demonstrate a low cost hydrogen storage material that has a capacity greater than 5.5 W%, is stable with hydrogen cycling, and possesses favorable thermodynamic and kinetic characteristics suitable for transportation applications. The approach to achieve these goals will be to combine two emerging hydrogen solid storage technologies and produce a superior hydrogen storage system.

Current approaches of hydrogen storage are compressed gas, liquid, or in the form of solid hydrogen. A solid hydrogen storage system is reliable, simple to engineer, and tremendously safe. Examples of solid hydrogen storage are metal hydrides, carbon (nanotubes, Fullerenes and activated carbon) or glass microspheres. Single wall porous carbon nanotubes (SWNT) have shown promise for hydrogen storage. Several research institutes and companies in the US and elsewhere are exploring the use of carbon nanotubes for hydrogen storage. Single wall nanotubes technology represents a new direction for solid hydrogen storage especially if these materials can store larger amounts of hydrogen at room temperature than does graphite alone. On another front a breakthrough has been achieved by developing new alanate complex compounds for hydrogen storage. Recently, it has been shown that alanate hydride complexes, such as sodium aluminum hydrides, could be modified to reversibly store large amount of hydrogen. Yet, neither of these systems (carbon nanotubes or alanates) has matured, especially for transportation applications.

Additional research is required to reach a product that has a stable hydrogen capacity with cycling and enhanced kinetics compatible with transportation applications. The modification of carbon nanotubes systems can hold the key to solving the hydrogen storage problem. Introducing a hydrogen bonding dopant can facilitate the adsorption and desorption of hydrogen by carbon SWNT, at practical temperatures and pressures. Dopants such as alanates can act as active sites in the carbon nanotubes forming surface clusters capable of bonding hydrogen with favorable thermodynamic and enhanced kinetics.

Westinghouse Savannah River Technology Center's (SRTC) approach can be divided along parallel but integrated tasks: material synthesis, thermodynamic characterization and elemental and spectroscopic analysis. The synthesis of material will be conducted using commercially available single wall nanotubes. Lithium aluminum hydride (LiAlH_4) and sodium aluminum hydride (NaAlH_4), as well as sodium boro-hydride (NaBH_4), will be used as dopants.

Task 1: Synthesis of Material

Several purification schemes will be applied to remove impurities from SWNT. For example, SWNT samples will be exposed to oxidative environment. Samples will be washed out in hydrocarbons and metal particles will be dissolved away with hydrochloric acid. The doping process will be performed on nanotubes purified as explained. The nanotubes will be added to a solvent containing a dissolved hydride. The amount of dissolved hydride (NaAlH_4 , LiAlH_4 or NaBH_4) will be varied to produce different levels of deponing material in the nanotubes.

Task 2: Thermodynamic and Energetic Characterization of Hydriding/Dehydriding

In order to determine the performance of these carbon nanotube systems preliminary Thermal Desorption Spectrum (TPD) will be performed on samples, using a thermovolumetric system. The rate of hydriding

and dehydriding will be obtained at fixed temperatures and pressures. The stability of the doped SWNT with cycling will be determined.

Task 3: Material Characterization and Elemental Analysis

After the purification of the SWNT samples the product will be characterized, using spectroscopic and elemental analysis. Hydrides such as NaAlH_4 , LiAlH_4 and NaBH_4 , will be purified by dissolution. The final product will be characterized using spectroscopy to assure high yield of pure material. Elemental analysis of the product will be conducted. The subsequent hydriding and dehydriding cycles will be monitored in parallel with elemental and spectroscopic analysis.

Doped Carbon Nanotubes for Hydrogen Storage Westinghouse Savannah River Technology Center						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Synthesis of Material						
Purification of SWNT		◆	◆	◆	◆	
Preparation of dopent		◆	◆	◆	◆	
Doping Process		◆	◆	◆	◆	
Thermodynamic Characterization						
Set up thermal desorption						
Hydriding and dehydriding					★	
Examine SWNT with cycling						◆
Material Analysis						
Spectroscopic analysis of product		◆	◆	◆		
Spectroscopic analysis of cycled samples					◆	
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Catalytically Enhanced Hydrogen Storage Systems – University of Hawaii

The University of Hawaii (UH) has developed methods of doping of sodium aluminum hydride, NaAlH_4 with titanium, zirconium and other catalysts such that: rapid dehydriding occurs at or below 100 °C; rehydriding requires less than 2 h; and 4.8 weight percent hydrogen can be repeatedly cycled through dehydriding/rehydriding. Thus, these materials appear to be on the threshold of practical viability as hydrogen carriers for onboard fuel cells. However, their dehydriding and/or rehydriding kinetics must be further in order to be utilized in practical onboard hydrogen storage systems. Unfortunately, the doping of NaAlH_4 with transition metal alkoxides and chlorides has now been explored extensively and this approach is nearly exhausted. Therefore, UH plans to screen new types of materials as catalysts for the reversible dehydriding of NaAlH_4 .

UH has also found a class of catalysts that could provide the key to a practical hydrogen storage system based on the reversible dehydrogenation of cycloalkanes to arenes. Such a system meets the criteria of low cost and high hydrogen density (~7.0 wt %). The PCP pincer complex, $\text{IrH}_2\{\text{C}_6\text{H}_3\text{-2,6-(CH}_2\text{P}^t\text{Bu}_2)_2\}$ is the first reported homogeneous catalysts for the dehydrogenation of cycloalkanes to arenes. Unlike the heterogeneous catalysts for this reaction, it shows appreciable activity at low concentrations at temperatures as low as 100 °C. They have also found that the pincer complex also catalyzes the hydrogenation of arenes to cycloalkanes under moderate (10 atm) pressures of hydrogen. The two-way, hydrogenation/dehydrogenation activity of the catalyst suggests its application in a hydrogen storage system. An additional incentive for the development of this type of catalyst within the context of the DOE Hydrogen Program has recently come to light. The University of Hawaii has found that the pincer catalyst is highly selective for the extrusion of hydrogen from linear alkanes to produce alpha olefins. Considering the large-scale production alpha olefins (50 million tons per year), it is possible that commercial processes for their production based on the dehydrogenation alkanes might also become an important source of hydrogen. This possibility is attractive in view of the increasing concerns about “carbon management” as hydrogen is produced in this catalytic system in concert with a high value commodity chemical rather than CO_2 . The major obstacle to the practical applications of the pincer catalyst is that pronounced product inhibition occurs after about 10% dehydrogenation of alkanes. In order eliminate this problem UH proposes to synthesize and test an improved catalyst, $\text{IrH}_2\{\text{C}_6\text{H}_3\text{-2,6-(CH}_2\text{As}^t\text{Bu}_2)_2\}$.

Task 1: Testing of Aluminum-Transition Metal Catalysts for the Reversible Dehydriding of NaAlH_4

The aluminum-transition metal alloys and the transition metal-aluminum hydrido complexes will be studied as catalysts for the reversible dehydriding of NaAlH_4 . Small amounts of the alloys and complexes will be introduced into bulk NaAlH_4 through ball milling techniques under an inert atmosphere. The dehydriding behavior of the hydride doped with these species will be screened by thermal programmed desorption studies as well as isothermal (100 and 150 °C) studies of their dehydriding and rehydriding kinetics by volumetric methods using a modified Sievert's type apparatus. Materials showing faster dehydriding and/or rehydriding kinetics than titanium or zirconium doped NaAlH_4 will be subjected to rate studies at 10 °C intervals over the range 80-150 °C in order to accurately determine the activation parameters of the dehydriding and rehydriding reactions through van't Hoff plots of the rate data.

Task 2: Solid State Nuclear Magnetic Resonance Spectroscopic Studies of the Reversible Dehydriding of NaAlH₄

These investigation will be conducted in collaboration with Prof. K. Kumashiro and Dr. W. Niemczura of the UH Department of Chemistry who are experts in solid state NMR spectroscopy. The bulk aluminum hydrides NaAlH₄ and Na₃AlH₆ will be studied by ²⁷Al NMR using magic angle spinning (MAS) and multiple quantum techniques that have been developed for the observation of quadrupolar nuclei in the solid state. UH will also prepare deuterated samples of the hydride for static, wide-line ²H NMR spectroscopic studies. These methods will give them detailed structural information about the hydrides. UH will then monitor the dehydriding and rehydriding processes by ²⁷Al and ²H NMR spectroscopy at temperatures ranging from 100-150 °C. The relative amounts of NaAlH₄ and Na₃AlH₆ throughout the process will be directly monitored through the observed signal intensities. Since each of the hydride species will be directly quantified over the course of the dehydriding and rehydriding processes, UH can determine the activation parameters for both of the dehydriding reactions and the reverse rehydriding reactions. Once refined, UH spectroscopic methods may allow the observation of the <2.0 % amount of the catalytic species and its identification upon comparison of its chemical shift and coupling constants to those of known species.

Task 3: Synthesis and Testing of an Arsino Pincer Catalyst for Reversible Alkane Dehydrogenation

UH plans to synthesize the arsino pincer complex. They have found that α,α -bis(arsino)-1,3-xylenes can be conveniently prepared from the reaction of α,α -dibromo-1,3-xylenes with borane adducts of dialkylarsine in THF solution at 25 °C. The hydrido chloride iridium complex, will be generated by refluxing the bis(arsine) with [Ir(COE)(μ -Cl)]₂ in toluene for 24 h. Reaction of the hydrido chloride complex with LiBEt₃H under an atmosphere of H₂ gives the target dihydride complex. The new pincer complex and all intermediate compounds will be characterized by ¹H, ¹³C, and ³¹P NMR spectroscopy and their purity verified by external elemental analysis. UH will quantify the catalytic activity of the arsino pincer complex for the dehydrogenation of cycloalkanes such as methylcyclohexane and linear alkanes such as *n*-undecane. They will also determine its catalytic activity for the hydrogenation of arenes, such as toluene, to the corresponding cycloalkane. The products resulting from the catalytic reactions will be identified using gas chromatography/mass spectrometer and quantified by standard gas chromatography.

Catalytically Enhanced Hydrogen Storage Systems
University of Hawaii

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Synthesis of transition metal-aluminum hydride complexes		◆				
Determine catalytic activity of aluminide alloys			★			
Development of solid state NMR methods			◆			
Synthesis of iridium arsino pincer complex		◆				
Determine catalytic activity of transition metal aluminum hydride complexes			◆			
Determine activation parameters by solid state NMR				◆		
Determine catalytic activity of arsino pincer complex				◆		

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Hydrogen Storage Development – Sandia National Laboratories

The purpose of this project is to develop and demonstrate improved hydride storage materials for fixed site, infrastructure and transportation uses. This project is integrated into Sandia's overall hydrogen utilization program, but also includes (a) collaborative efforts with other hydrogen program participants, (b) other university and industrial partners to demonstrate storage system integration with fuel cells and other applications, and (c) participation in International Energy Agency Annex 12, finishing this year, and Annex 17 beginning this year. The IEA work provides a mechanism for collaborating with researchers in Canada, Europe and Japan, and an international overview to the state-of-the-art in hydride development. Sandia has also participated in the Hydrogen Program educational outreach activities and plan to continue supporting these efforts.

The work has three main objectives: (1) the development of improved hydride materials, particularly lighter weight hydrides for vehicular applications, (2) the development of improved hydride bed fabrication methods, and (3) provide advanced materials and systems to engineering and industrial collaborative programs. This year, the project is organized into the following five tasks:

Task 1: Light Weight Hydride Development

The work will continue this year with a focus in two areas – (1) improving the engineering properties for practical storage applications, and (2) understanding the physical and chemical mechanisms of hydrogen release and absorption in order to make further advances in light weight storage materials. The approach will be as follows:

- Continued collaboration with the University of Hawaii, where Sandia will emphasize engineering properties and the Hawaii investigators will emphasize catalyst development.
- Sandia's study of engineering properties will be complemented by efforts to develop improved material preparation methods, including catalyst processing, with the aim of optimizing performance.
- Mechanistic studies of the reaction processes using gas-phase measurements and characterization of the material by electron microscopy and spectroscopic techniques.
- Complete testing and document safety studies on Na-alanate.
- Begin investigating substituted alanates of the form $\text{Na}_{1-x}\text{X}_x\text{Al}_{1-y}\text{Y}_y\text{H}_4$, where X and Y are elements other than Na and Al.
- Summarize the work to date with a series of papers and presentations at the Metal-Hydrogen 2000 Conference.

Sandia will also complete a short-term study on an alternative to complex hydrides, carbon-based storage media. Published results on carbon nanotubes and carbon-catalyst mixtures suggest these materials are also promising hydrogen storage candidates. Quantitatively, however, capacity values and temperature behavior vary considerably between investigators. In FY00, Sandia contracted with Prof. C-H. Kiang, UCLA, to provide carbon nanotubes prepared by the same processes as reported in the literature. The objective was to apply Sandia's experimental apparatus and experience in accurate gas-phase measurements to provide an independent examination of these published values. They have begun absorption and desorption measurements to determine capacity and kinetic properties over a range of temperatures and pressures. Unless exceptional results are found, this work is considered to be a short-term project and is expected to be completed by the first quarter of FY01.

Task 2: Mine Locomotive Powerplant

This project will result in the development and evaluation of a fuel cell-powered mining vehicle, specifically, a 4-5 ton electric drive locomotive designed for use in mines and tunneling operations. The project is a joint venture between U.S.D.O.E., CANMET (Canada) and private industry in Canada and the U.S. Sandia's role is the development and fabrication of a fuel cell-hydride powerplant for the vehicle. However, Sandia's engineering effort has been significantly increased beyond the original plans because of two factors – (a) unavailability of the SRL hydride beds from the hydrogen bus and (b) delivery by Nuvera of fuel cell stacks without the balance-of-plant equipment required for their operation. Sandia's plans for completing this project are as follows:

Sub-Task 2-1: Powerplant completion and integration with locomotive.

The power plant assembly, as per the initial designs, will be supplied for use in the MINExpo 2000 display scheduled for Oct. 2000. The late delivery of the fuel cell stacks (Sept. 2000), however, does not allow sufficient time for testing and characterizing the powerplant performance prior to the exposition. Following the MINExpo display, testing and evaluation of the powerplant will be completed at Sandia, then the assembly will be shipped to Atlas Copco Wagner for integration with the locomotive. Sandia will also supply engineering consultation as needed during this phase. An operational procedures document will be completed in cooperation with Atlas Copco Wagner and R.A. Hershey, (the locomotive manufacturer) and a refueling manifold and refueling procedure document will be completed.

Sub-Task 2-2: Evaluation of refueling options

The next phase of this work is concerned with evaluating the performance of the vehicle and addressing operational issues. Sandia's role will be focused on refueling – options, procedures, and equipment. This work will include fabrication of a second hydride bed to evaluate refueling directly from one bed to another versus exchanging beds using an external refueling source. Sandia will also participate in the overall testing and evaluation through consultation, maintenance and analysis of results.

Task 3: High Pressure Hydrogen Tank Testing

This project was started last year to provide visual and quantitative information to OEM's, regulatory agencies and the public regarding the consequences of failures in on-board high pressure hydrogen tanks. In response to criticisms brought out during the program review, the test matrix and test details were modified, using inputs from the oversight committee formed this year and from consultants. Original planning called for completion of the project approximately the first quarter of FY01.

Task 4: IEA Annexes 12 and 17

This task includes all additional IEA activities outside of the hydride development work described in Task 2, and consists of the following subtasks:

Sub-Task 4-1: Dr. Gary Sandrock, SunaTech, Inc., as Operating Agent for Annex 12

Annex 12 is essentially completed after 3 years. This years activities will consist of closing out all projects within the Annex and writing of the final report.

Sub-Task 4-2: Dr. Gary Sandrock, SunaTech, Inc., as Operating Agent for Annex 17

Sub-Task 4-3: Continue to expand the online database

As of the beginning of FY01, there are six databases operational on the server system. This server is a unique, powerful and accessible source of information on state-of-the-art materials, material properties and world-wide research activities.

Sub-Task 4-4: Additional Sandia activities in support of Annex 17

These other activities include maintaining the online database server and participating as partners in other projects within Annex 17.

Task 5: Educational Outreach

Sandia will continue to participate in demonstrations at schools and at teachers workshops such activities as needed by the educational outreach coordinator. Furthermore, Sandia will maintain the fuel cell powered car supplied to a school in 1999 through periodic maintenance and repairs as needed.

Hydrogen Storage Development Sandia National Laboratories						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Lightweight Hydride Development						
MH2000 Papers		◆				
Carbon evaluations			◆			
Safety Studies					◆	
Optimize TiCl ₃ catalyst				◆		
Mine Locomotive Powerplant						
Mine expo display		★				
Testing and documentation				◆		
Refueling study completed					◆	
High Pressure Tank Testing						
Complete project			★			
IEA						
Begin Annex 17		★				

FY 2001 Begins October 1, 2000

Hydrogen Storage in Polymer-dispersed Metal Hydrides – United Technologies Research Center

Hydrogen storage has been intensively studied for many decades and present technologies still do not meet the automotive goals of a 5.5 wt. % gravimetric capacity and a volumetric capacity of 60 kg/m³. Meeting both volumetric and gravimetric capacity goals with one technology provides an extremely difficult technical challenge. Some hydrogen-storage methods include: compressed gas storage in large tanks or glass microspheres, liquid hydrogen, cryogenic adsorption, storage in carbon nanotubes, nanofibers, or fullerenes, chemical storage (such as liquid organic hydrides), and metal hydride storage. Metal hydrides generally demonstrate high volumetric capacity, but low gravimetric capacity. United Technologies Research Center (UTRC) proposed a completely novel approach to improve the gravimetric and volumetric storage capacity of metal hydrides, by dispersing metal-hydrides in active polymer supports. In this program, UTRC proposes to investigate polymer-dispersed metal hydrides for hydrogen storage, and intends to: 1) demonstrate that polymer-dispersed metal hydrides can meet the 5.5 wt. % DOE goal for hydrogen storage, and 2) evaluate the systems impact, including weight, volume, cost, and thermal requirements of this approach.

Polymer-dispersed metal hydrides offer a unique opportunity to enhance the storage capacity of available and future metal hydride materials. Improvements in gravimetric storage capacity by factors of 2-5 are anticipated relative to the non-dispersed metal hydrides. In addition, dehydriding temperatures may be reduced, potentially enabling automotive waste heat to be used to dissociate the hydride. Dispersing the metal hydride in a support material is expected to benefit the stability of metal hydride materials as well. Development of polymer-dispersed metal-hydride technology could significantly benefit our economy, environment, and competitiveness by enabling fuel cell powered vehicles. In addition, battery technology could improve as a result of this program, resulting in lower-cost, longer-lasting, rechargeable batteries. The proposed technology may also apply to new alloy metal hydrides material as they are developed, allowing even higher-capacity storage systems to emerge.

Task 1: Material and Method Selection

Various polymers, metal hydrides and mixing methods were selected, and approximately 10 samples were prepared from various combinations of polymer, metal hydride, and method.

Task 2: Characterization of Basic Mechanisms

In this Task, experimental work will be performed to quantify the hydrogen storage capacity of various polymer-containing samples, and to elucidate the mechanisms that control hydrogen storage in PDMH materials.

Task 3: System Characterization to Achieve Project Goals

Data obtained in Task 2 will be used to perform a preliminary systems analysis to characterize PDMH hydrogen-storage systems. System weight, volume, thermal, and pressure requirements will be analyzed, and a preliminary cost analysis will be performed for a 50 kW fuel cell system.

Task 4: Phase 2 Plan Development

This Task will incorporate information gained from Tasks 1-3 to develop a comprehensive plan to create PDMH hydrogen storage systems consistent with the DOE hydrogen program goals. This activity will

require a down-selection, based on materials and methods limitations (i.e. storage capacity, temperature and pressure characteristics, fabrication ease, materials availability, etc.), as well as UTRC's ability to develop the technology. UTRC will then define a Phase 2 R&D strategy, most likely based on a scale-up of synthesis techniques and larger-scale performance measurements. The Phase 2 plan will attempt to identify and demonstrate a materials and delivery system, at a reasonable scale to allow a more detailed assessment of the technology.

Task 5: Reporting

This Task includes monthly updates, a final report summarizing the results of Phase 1, and a detailed Phase 2 Program Plan.

Hydrogen Storage in Polymer-Dispersed Metal Hydrides United Technologies Research Center						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Material and Method Selection	◆					
Characterization of Basic Mechanisms						
Synthesis of PDMH samples				★		
Characterization of PDMH samples		◆				
System Characterization to Achieve Project Goals						
System design				◆		
Cost analysis				◆		
Phase 2 Plan Development				◆		
Final Report					★	

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PHYSICAL STORAGE

Vehicular Hydrogen Storage Using Lightweight Tanks – Lawrence Livermore National Laboratory

Advanced composite hydrogen tanks are undergoing rapid evolution. This proposal advances hydrogen tankage beyond the current state-of-the-art in materials, processes, and cost, as well as providing tanks for demonstration vehicles and supporting improved safety standards.

Research of tank technologies is proposed that might merit commercialization in roughly three years. The proposed research has elicited vigorous interest from industrial partners, and should result in safer, denser, less expensive, as well as lighter-weight hydrogen storage for vehicles. Lower cost tanks will result from more efficient composite utilization and advances in thin liners (with regard to which numerous advances have been made over the past two years), as well as process and materials research that should establish the feasibility of blow-molded liners.

Near-term generation tanks can deliver roughly a fifty percent driving range improvement over existing products for a given hydrogen storage volume on-board a specific vehicle. Very little new technology is required for this performance advance; the DOE solicitation process has been employed to demonstrate what is currently possible in safe, Type IV (plastic-lined composite) hydrogen tanks. The LLNL tankage development team has been adapting and transferring aerospace technology into this arena.

Recently LLNL set a weight record for hydrogen tank technology: 11.3% percent hydrogen stored by weight in a tank technology with sufficient cycle life for vehicular applications. Although much prior art was applicable to engineering on the weight frontier, very advanced design and testing techniques could not locate the failure mechanism that claimed 7% of predicted fiber failure strain, strength which might otherwise be applicable to cost and weight reduction. Future research efforts will be directed at identifying the mechanisms responsible for this performance loss.

The proposed tasks for FY 2001 includes two tasks intended to improve current safety certification standards. In addition to dealing with U. S. regulations, LLNL will also address international concerns. In addition, a major thrust of the proposed effort in FY 2001 will be to improve the density of compressed hydrogen storage by research at 10,000 psi storage pressure. Material-related degradation issues at pressures above the yield stress of liner and seal materials (materials which have been proven to be acceptable for containment of hydrogen at 5,000 psi) will be researched. In the case of composite overwrapping, liner prototyping, burst testing, and some material testing LLNL must rely on subcontractors to execute portions of research plans. Tasks have been planned to incorporate knowledge gained from those subcontracts to make the “generation-after-next” (e.g., 3 years from commercialization) tanks using highly economical blow-molding by prototyping 4” diameter tanks (applicable to motorcycles).

Project tasks depend on final funding level for FY 2001, currently in negotiation.

Task 1: Work with Industry to Adopt Embedded Electronics Concepts for Tanks

LLNL will work with industry to understand and adopt embedded electronics (continuing the “Smart Tank” project) that will significantly improve the safety and operability of vehicular hydrogen tankage. They will apply engineering and economic principles developed in the previous DOE project, as well as preferred solutions from important manufacturers and infrastructure vendors. They will study design,

features, and market niche alternatives before advocating a new standard that will enable safer interoperability of “Smart Tanks”.

Task 2: Certify Tankage for Operation on Vehicles (e.g. NGV2 standards modified for H₂)

LLNL will technically direct current and anticipated DOE contracts with industry to help them reduce risk through judicious testing and design choices. Knowledge will be transferred between contractors and the results of research will be made available in order to increase probability of delivering safety-certified tanks for DOE demonstration projects.

Task 3: Modify Tank Designs for Easy Manufacturability

This task will require the redesign, prototyping, and burst-testing of advanced tanks at an affordable 4” diameter size. The new size for integrated tank development will be relevant for scooters and motorcycles, while allowing exploration of process variables with sufficient quantities of test articles. LLNL will work to encourage industry to adopt advanced tankage designs.

Task 4: Work with Industry to Develop Concepts to Reduce the Cost of Hydrogen Tankage

Investigate blow-moldable liner materials by fabricating, strain testing, and permeation testing the obvious single and multilayer material candidates suitable for replacing the more limited (and costly) list of rotationally-moldable liner materials.

Task 5: Work with Industry to Develop Advanced Higher Pressure Tanks

LLNL will work with industry to develop advanced hydrogen tankage with service pressure ratings up to 10,000 psi (69 Mpa). They will investigate relevant materials properties (permeation, cyclic fatigue) for components of tanks which must function above their yield stresses using small nonplanar (e.g. sections of ~4” diameter cylinders) samples in a new apparatus capable of cycling. Moisture and chemical attack issues will be explored if suitable candidate materials are found.

Task 6: Work with Industry and Academia to Demonstrate Lightweight Hydrogen Tanks on Fuel Cell Vehicles

Engineering issues will be analyzed. LLNL will maintain close contact with the relevant institutions and companies, and promote the dissemination of technical information in this area as well as education of students. This will be done in a timely fashion in order to maximize the probability of success on at least three DOE demonstration projects that seek to integrate DOE supplied tanks (developed under Task 2 above).

Task 7: Suggest Modifications to Hydrogen Tank Standards and Codes

LLNL will collect input, draft, and advocate a U. S. standard to restart the safety certification debate from a standpoint based on the actual risks of hydrogen. They will help advocate the new U. S. standard aggressively in the international arena involved with the ongoing ISO TC197 process (with collaborators from the NHA, NASA, German colleagues, and the U. S. Compressed Gas Association).

Vehicular Hydrogen Storage Using Lightweight Tanks
Lawrence Livermore National Laboratory

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Work with Industry to Adopt Embedded Electronics Concepts for Tanks						
Apply sound engineering and economics principles for "smart tanks"			◆			
Certify Tankage for Operation on Vehicles (e.g. NGV2 standards modified for H₂)						
Technically direct multicontractor efforts to develop tanks for demonstration projects			★		◆	
Modify Tank Designs for Easy Manufacturability						
Redesign, prototype, and burst test 4" diameter tanks				◆		
Work with Industry to Develop Advanced Higher Pressure Tanks						
Develop tanks with service pressure ratings up to 10,000 psi			◆			
Work with Industry and Academia to Demonstrate Lightweight Hydrogen Tanks on Fuel Cell Vehicles						
Coordinate efforts leading to demonstrations on fuel cells						★
Suggest Modifications to Hydrogen Tank Standards and Codes						
Advocate new U.S. and international standards appropriate for hydrogen storage					◆	

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Advanced Thermal Hydrogen Compression - Ergenics, Inc.

One obstacle impeding the development of economical hydrogen production, storage and utilization is hydrogen compression. Large mechanical hydrogen compressors have a high capital cost, consume substantial amounts of energy and require frequent maintenance. Hydrogen compression becomes more difficult when hydrogen is produced from renewable energy resources. Generally, these hydrogen production methods produce hydrogen at atmospheric pressure; boosting pressure from atmospheric to the 5000 psia pressure being considered for transportation applications is more difficult and requires more complex equipment than large compressors used today.

Ergenics, Inc. has developed a novel thermal hydrogen compressor¹ that may offer advantages for compressing hydrogen produced from renewable resources using advanced production techniques. Two recent innovations strongly suggest that thermal compressors can be used for non-pure hydrogen streams likely to result from advanced production methods. The first involves a combination of three purification processes that permit the absorption of impure hydrogen streams by hydride alloys. The second is a modular alloy bed design that permits rapid hydrogen absorption kinetics, enabling a reduction in compressor size with an associated reduction in capital cost.

The long term goal of this project is to develop a thermal hydrogen compressor that operates in conjunction with advanced hydrogen production technologies and improves the efficiency and economics of the compression process.

The plan for FY 2001 is to demonstrate a pilot-scale thermal compressor operating on impure hydrogen. The effectiveness of three purification processes will be monitored and operating limits will be experimentally determined. In the case of impurities that can adversely effect fuel cell operation (e.g. nitrogen, CO), outlet hydrogen purity will be monitored to verify the degree to which a thermal compressor can perform the dual function of compressing and purifying hydrogen. This will allow the evaluation of trade-offs between hydrogen purity and compressor and fuel cell operating efficiencies necessary for the design and integration of full-scale systems. At the conclusion of the FY 2001 effort, the performance expected from large advanced thermal hydrogen compressors will be understood, substantially reducing the risks associated with a full scale demonstration of this exceptional technology.

Task 1: Single Stage Thermal Compressor

Build a single stage thermal compressor that uses miniature hydride heat exchanger technology and includes three purification technologies. The purification technologies are passive purification for oxygen and water, inert gas purification via automatic venting, and elevated temperature desorption for CO and CO₂.

Task 2: Assemble Compressor Test Apparatus

Assemble a compressor test apparatus that can simulate hydrogen inlet compositions expected from advanced hydrogen production technologies and can monitor compressor performance. Impurities include air, water vapor, oxygen, nitrogen, CO and CO₂.

¹ Ergenics' thermal compressor is an absorption based system that uses the properties of reversible metal hydride alloys. Hydrogen is absorbed into an alloy bed at ambient temperature and is desorbed at elevated pressure when the bed is heated with hot water.

Task 3: Test Thermal Compressor

Test the thermal compressor over a range of hydrogen compositions. Inlet impurity levels will be varied to determine threshold contamination levels (levels at which compressor performance is affected). Outlet hydrogen pressure, flow rate and purity will be monitored.

Task 4: Evaluate Application of Thermal Hydrogen Compression

Evaluate the application of thermal hydrogen compression to various advanced hydrogen production methods.

Task 5: Final Report

Summarize FY 2001 activities in a Final Report with recommendations for future project activities.

Advanced Thermal Hydrogen Compression Ergenics, Inc.						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Build a single state thermal compressor			◆			
Assemble a compressor test apparatus				★		
Test the thermal compressor					◆	
Evaluate the application of thermal hydrogen compression to various advanced hydrogen production methods						◆
Summarize FY 2001 activities in a final report						◆
FY 2001 Begins October 1, 2000						

3.1.3 Hydrogen Utilization Research Projects

Utilization of hydrogen as an energy source occurs typically either via an electrochemical process such as in a fuel cell or by a combustion process. In addition, the use of hydrogen necessitates the ability to detect its presence in the event of leaks. The Hydrogen Program effort also supports R&D in the area of hydrogen sensors. This section, summarized in Table 3.4, is categorized accordingly.

Table 3.4		
Hydrogen Utilization Research		
Goal: Develop fuel cell and reversible fuel cell technologies as an efficient low-cost means of converting hydrogen into electric power.		
Category	Project	Researcher
<i>Fuel Cells</i>	Small Battery/ Fuel Cell Alternative Technology Development	Los Alamos National Laboratory
	Low Cost Reversible Fuel Cell System	Technology Management, Inc.
	Hydrogen Delivery System to PEM Fuel Cell	New Jersey Department of Transportation
	Gallium Nitride Integrated Gas/Temperature Sensors for Fuel Cell System Monitoring for H ₂ and CO	Peterson Ridge, LLC
	Design and Development of New NanoEngineering Glass-Ceramic Proton Conducting Membranes (GCPCMs) for High Performance H ₂ -O ₂ Proton Exchange Fuel Cells	Iowa State University
<i>Internal Combustion Engines/ Turbines</i>	Internal Combustion Engines Research and Development	Sandia National Laboratories
	Reduced Turbine Emissions Using Hydrogen-Enriched Fuels	Sandia National Laboratories
	Hydrogen/Natural Gas Blends	NRG Technologies
<i>Hydrogen Safety</i>	Interfacial Stability of Thin Film Hydrogen Sensors	National Renewable Energy Laboratory
	Integrated Micro-Machined Hydrogen Gas Sensors	Advanced Technology Materials, Inc.
	Analysis of Codes and Standards Requirements	University of Miami
	Hydrogen Infrastructure Activities	National Renewable Energy Laboratory
	High Efficiency Steam Electrolyzer	Lawrence Livermore National Laboratory

FUEL CELLS

Small Battery/Fuel Cell Alternative Technology Development – Los Alamos National Laboratory

Depending upon the fuel storage technology, fuel cell systems can provide substantially higher energy densities than similar-sized battery packs. Correspondingly, interest in fuel cells for portable power applications is rapidly increasing and now global electronics companies are pursuing the possibilities. In this program, Los Alamos National Laboratory (LANL) has been partnered with Enable Fuel Cell Corporation (a subsidiary of DCH Technology, Inc.) in a Cooperative Research and Development Agreement (CRADA) to develop a unique low-power portable fuel cell and system for applications that require a combination of reliability, simplicity and low-cost. The advantage of this fuel cell system over current competing designs is that it does not require the use of peripherals such as cooling or reactant flow fans and can operate effectively with no active humidification, no active cooling, and no pressurization or forced flow of the cathode air. The system is inherently stable and self-regulating. A passive scheme is used that relies on diffusion limited oxygen access to maintain a positive water balance. The oxygen in the air must diffuse into the stack from the periphery of the flow-field plates. For this reason the stack is often described as "air-breathing." Given that the oxygen must diffuse in, twice as much water (as there are two molecules formed per O₂ that reacts) must diffuse out to maintain an even balance. While it first appears that a surplus of water is obtained, the fuel cell stacks quickly heat up and the water removal is greatly facilitated. Overall, the balance remains fairly even such that the polymer electrolyte membranes do not dry out, even at relatively high continuous operation temperatures (+60 °C). Thus, the diffusion supply scheme results in simple stacks with reliable and stable performance. Since the oxygen needs to diffuse in from the periphery of the cathode flow-field plate, the fuel cell assumes a cylindrical configuration that utilizes circular flow-field plates with an annular hydrogen feed manifold and a single tie-bolt extending up through the central axis of the stack. With this geometry, the hydrogen supply to the unit cells is radially outward, and the air supply is from the periphery inward. This configuration facilitates performance (e.g., maximizes cooling surface area, air access, etc.) and is very simple for cost considerations (low parts count, all parts are radially symmetrical, etc.). To operate this type of fuel cell stack only a low pressure hydrogen supply is required which can be provided from a pressurized source (such as metal hydride canisters) via a passive compact low-pressure regulator.

Where LANL primarily differs with most other portable power efforts is their belief that success will require the development of extremely simple fuel cells and systems, as simplicity beneficially influences cost, durability and reliability. Hence, the long-term goal is to develop commercially competitive fuel cell power sources for electronics and other battery-type applications.

Task 1: Air-breather System Refinement

LANL plans to continue collaborating with Enable FCC in developing air-breather technology. As the fundamentals and optimal designs become better understood and more functional, opportunities arise to implement newer ideas and approaches that will bring the air-breather to the next technical levels. As such, some elements of the development effort are somewhat open-ended as the product and understanding evolve.

One of the difficulties is to obtain a reasonable fraction of active area with such small diameters because so much of the plate area is lost to seals, the tie bolt and the hydrogen feed region. Although the current densities are even higher than the larger stacks (as expected), further performance increases should be

readily attainable as the various elements are brought together and optimized. Correspondingly, one of the air-breather subtasks is to refine and improve the small air-breather design and performance.

Task 2: Portable Hydrogen Storage

Attention will be directed toward the hydrogen supply for the fuel cells. In this new aspect of the portable fuel cell effort, LANL intends to collaborate with Enable FCC and others to help develop and demonstrate portable storage technologies. Some of the challenges and opportunities inherent in a portable unit for commercial applications are very different than conventional storage requirements. As such, fairly conventional chemical hydrides that are not particularly attractive for largescale applications are possibly advantageous for portable systems. Thus, LANL are not trying to develop new chemistries so much as to effectively and inexpensively adapt existing approaches and repackage them for portable power.

Task 3: Alternate Portable FC System Development

One possible approach to the fuel storage problem that is particularly well suited for an alternative portable fuel cell system is actually fairly old and was also briefly considered at LANL more than 10 years ago, but was impractical at the time. Since, some technological innovations, particularly those developed elsewhere in LANL, may make the approach possible. This task will consist of this explorative development. While highly speculative, the system advantages are significant, if successful, for portable power and possibly other applications.

Small Battery/Fuel Cell Alternative Technology Development Los Alamos National Laboratory

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Air-Breather System Refinement						
Alternative materials development/testing						◆
System refinement						◆
Watt-level stack optimization						◆
Portable Hydrogen Storage						
Hydride material investigations				◆		
System development and demonstration					◆	
Alternate Portable FC System Development						
Component development					◆	
Proof-of-concept demonstration				★		
System development						◆

FY 2001 Begins October 1, 2000

Low Cost Reversible Fuel Cell System –Technology Management, Inc.

Off grid, renewable based energy supply systems using either wind turbines or solar photovoltaic generation normally require both significant electrical energy storage (currently by deep cycle lead acid batteries) and auxiliary generation from fossil fuel (currently by an engine-generator). Significant improvements in both storage and auxiliary generation are desired for both lead acid batteries and engine generators. Lead acid batteries have poor storage efficiencies and high life cycle costs. Engine generators have poor fuel efficiency, high life cycle costs, high noise, and high pollution.

Technology Management Inc. (TMI) has demonstrated solid oxide fuel cells and small stacks operating reversibly on hydrogen + steam/oxygen. TMI has also demonstrated SOFC systems operating on reformed hydrocarbons/air. Many of these cells and stacks have exhibited relatively low total polarization's in both fuel cell and electrolysis modes at practical current densities. Considerable development work is still needed to extend the useful life of these stacks and to improve the large seals required.

TMI has studied conceptual designs for stacks and systems using modifications of its existing solid oxide technology which offer the promise of high efficiencies for both energy storage (H_2/O_2) and hydrocarbon/air generation.

Phase 1 of this project was completed in September 2000. Phase 2 focuses on developing reversible fuel cell/electrolyzer stacks with emphasis on improved performance. Stacks would be applicable to high efficiency systems of both the energy storage type (using $H_2/H_2O/O_2$) and the power generation type (using fuel/air). Stacks are the heart of the proposed new systems and are currently seen as the area of highest technical risk. A subsequent Phase 3 would extend engineering work to produce detailed designs, followed by the fabrication and demonstration of working small complete systems of both types. The Phase 2 proposed tasks include:

Task 1: Design/Build Test Systems

This task will involve demonstrating and characterizing the TMI reversible fuel cell/electrolyzer technology.

Task 2: Seal Development

This task will establish viable sealing in the fuel cell/electrolyzer stack.

Task 3: Stack Demonstration

Stack demonstrations will occur in both storage battery mode and fuel cell mode to establish system efficiencies (energy storage efficiency over 80% and fuel cell LHV efficiency over 50%) and stability.

Task 4: Report and Phase 3 Proposal

This will summarize all work the performed and propose detailed engineering studies and designs for both the storage battery and the high-efficiency fuel cell systems and follow-on laboratory development work on stacks.

**Low Cost Reversible Fuel Cell System
Technology Management, Inc.**

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Stack test stands		◆				
Seal development				★		
Stack development and testing				◆		★
Final report and Phase 3 proposal						◆

FY 2001 Begins October 1, 2000

Hydrogen Delivery System to PEM Fuel Cell – New Jersey Department of Transportation

NJDOT retained Rutgers Center for Advanced Infrastructure and Technology (CAIT) to administer and manage contracts concerning development of a hydrogen generator system for PEM fuel cells. CAIT has subcontracted Millennium Cell, Inc. to develop an aqueous borohydride hydrogen delivery system and H-Power, Inc. to manufacture the PEM fuel cells.

Millennium Cell has produced a hydrogen generator using the surface catalytic reaction of ruthenium hydrolyzing sodium borohydride on contact.

The generator pumps an aqueous alkaline sodium borohydride solution from a tank through a cylindrical catalytic reaction chamber where the borohydride solution is hydrolyzed. Hydrogen and solution are expelled from the reaction chamber into a cylindrical storage tank. The hydrogen exits through a stainless steel tube as the hydrogen for the fuel cell. The hydrolyzed borohydride solution remains in storage tank.

Task 1: Identify Contaminates in Hydrogen Stream

Contaminates can damage the fuel cell membrane.

Task 2: Devise Approach to Remove Contaminates

Task 3: Tests to Verify Contaminates are Removed

Task 4: Integrate Hydrogen Generator with Fuel Cell and Test System

Task 5: Prepare Final Report

Hydrogen Delivery System to PEM Fuel Cell New Jersey Department of Transportation						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Identify contaminants in hydrogen stream	◆					
Devise approach to remove contaminants	◆					
Tests to verify contaminants are removed	◆					
Integrate hydrogen generator with fuel cell and test system	★					
Prepare final report		◆				
FY 2001 Begins October 1, 2000						

Gallium Nitride Integrated Gas/Temperature Sensors for Fuel Cell System Monitoring for Hydrogen and Carbon Monoxide -Peterson Ridge, Llc

The electrodes in solid polymer electrolyte fuel cell systems require hydrogen fuel free from carbon monoxide (CO), or the platinum electrodes are poisoned and fuel efficiency is degraded. Steam reforming of hydrocarbon fuels produces a mix of hydrogen, carbon dioxide and enough by product CO to poison the electrodes. Preferential oxidation (PROX) of CO to reduce this contaminant is accomplished over a noble metal catalyst typically platinum by adding oxygen to the hydrogen fuel upstream of the PROX catalyst. An inexpensive monitor to confirm the PROX catalyst efficiency and ultimately control the PROX system conditions is useful if not necessary to avoid the risk that PROX catalyst degradation could lead to reduced fuel efficiency or failure of the fuel cell due to contaminated hydrogen. Since the environment for a PROX monitor is rich in hydrogen, the problem is developing a sensor sensitive enough to monitor carbon monoxide at high temperature without the sensor output being dominated by hydrogen or temperature.

Peterson Ridge is exploring an approach combining the advantages of the sensing capabilities of the catalytic metal gate with a wide bandgap gan semiconductor metal semiconductor field effect transistor (mesfet) and modulation doped field effect transistor (modfet) transducers for high temperature measurement of carbon monoxide in hydrogen. The choice of the catalytic metals for the device is based on the metals used in fet detectors for lower temperature applications and based on data for metals used in the three-way automobile catalytic converter: platinum, palladium/silver and rhodium.

Task 1: Sensor Fabrication and Packaging Complete

Task 2: Complete Sensitivity Testing

Task 3 Phase I Report & Phase II Proposal Delivered

Task 4: Complete Prototype Development Plan

The plan includes: a sensor and package upgrade along with system design for a field demonstration program, a technology transfer of the fabrication process from the University of Utah to a commercial GaN foundry.

Task 5: Complete Prototype Preliminary Design

Redesign of the sensor to include a dielectric layer under the metal gate electrode is necessary to reduce gate leakage current. Ruggedized packaging for a field demonstration program will be designed.

Task 6: Fabrication, Testing and Refabrication Complete

A long-term program of redesigning and fabricating sensors as well as laboratory testing and possible refabrication will be focused on a rugged sensor for field demonstration and commercial purposes.

Task 7: Demonstration Development Plan Complete

The demonstration program will involve fuel cell manufacturers who have shown an interest in the sensor.

Task 8: Outsource 2nd Generation Fabrication

Commercial manufacturing is the goal of this task.

Task 9: High Temperature Probe Assembly Complete

The probe assembly sensor combination will be made to fit standard tube and pipe fittings to be determined after negotiating with fuel cell manufacturers on the demonstration program.

Task 10: Complete Test Article Assembly and Test

The test articles including sensor probe, data acquisition and communication modules will be assembled and calibrated in the laboratory prior to installation in the field.

Task 11: Mfg. Documentation Complete

Documentation will be necessary and sufficient for transfer and outsourcing the sensor fabrication process as well as for system integration and assembly.

Task 12: Begin Demonstration Roll Out and Delivery

Test articles will be delivered and installed on fuel cells at each of the five to ten fuel cell manufacturers in the program.

Task 13: Field Demonstration & Evaluation Complete

The test article will be monitored remotely for continuous evaluation during the program.

**Gallium Nitride Integrated Gas/Temperature Sensors for Fuel Cell System Monitoring for Hydrogen and Carbon Monoxide
Peterson Ridge, LLC.**

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Sensor fabrication and packaging complete	★					
Complete sensitivity testing	◆					
Phase I report and Phase II proposal delivered		◆				
Complete prototype development plan		◆				
Complete prototype preliminary design		◆				
Fabrication, testing and rework complete			◆			
Demonstration plan complete			◆			
Outsourced fabrication contracted			◆			
High temperature probe assembly complete				◆		
Complete test article assembly and test					◆	
Mfg. Documentation complete				◆		
Begin demonstration roll out and delivery					★	
Field demonstration and evaluation complete						◆

FY 2001 Begins October 1, 2000

Design and Development of New Nanoengineering Glass-Ceramic Proton Conducting Membranes (GCPCMs) for High Performance H₂-O₂ Proton Exchange Fuel Cells – Iowa State University

An entirely new class of high-temperature, anhydrous, fast proton conducting (FPC) membranes will be designed and developed for use in new high-performance hydrogen–oxygen fuel cells. These new NanoEngineered glass-ceramic proton conducting membranes (GCPCMs) are expected to yield high proton conductivities, $>10^{-1}(\text{ cm})^{-1}$ between 100 and 300°C, excellent thermal stability up to 300°C, superior electrochemical and chemical stability, and zero fuel cross-over diffusion. These high-performance GCPCMs are expected to solve many if not all of the critical problems currently seen in the proton conducting membrane of choice Nafion™ used in polymer electrolyte membrane (PEM) fuel cells. GCPCMs are expected to yield higher conductivities, greater chemical, and electrochemical stabilities, higher temperature operation, and zero fuel cross-cover compared to Nafion™.

In this project, FPC chalcogenide glasses already being developed in the Principal Investigator's (PIs) laboratory will be processed by well-known glass-ceramic processing routes to yield GCPCMs with controlled and optimized nanostructures. In a typical experiment, a hydrogen iodide- and hydrogen sulfide- doped boron trisulfide glass will be cast as a thin film, cooled to a nucleation temperature just below the softening point of the glass, held for a period of time to create nuclei of the FPC phase, and then heated to a growth temperature just above T_g to crystallize the glass to a predetermined and optimized crystallite size and volume fraction of the FPC phase.

Once processed, the GCPCMs will be characterized. Their thermal, electrical, and physical properties will be determined, as will their atomic structures.

Task 1: Literature Review

A critical review recent and established literature in the area of proton conducting glasses, ceramics, and glass-ceramics will be preformed to determine the state-of-the-art in these areas. A preliminary review has already been conducted and while some poorly conducting oxide glasses are know, no chalcogenide glasses or glass ceramics are known. A more thorough and critical review will determine the exact state of knowledge in this field.

Task 2: Hiring of Research Staff

One undergraduate research assistant, URA, one graduate research assistant, GRA, and one post-doctoral research associate, PDRA have been budgeted and funded on the project. The URA will be hired by announcing the position on the ISU campus in the College of Engineering to all qualified undergraduate engineering students. The GRA will be hired by offering the position to all interested and qualified incoming graduate students to the MSE department for the 2000/20001 academic year. The PDRA will be hired by soliciting applications at upcoming national meetings, the American Ceramic Society meeting for example, and by mail and e-mail announcement of the availability of the position to colleagues and faculty worldwide who are active in the area of ion conducting glasses.

Task 3: Synthesis of Proton Conducting Glasses

B₂S₃-based glasses will be doped with H₂S into the melt by gas bubbling. In a typical process, a melt of ~ 10 grams of B₂S₃ held in a chemically inert carbon crucible at a processing temperature of 500 to 800°C will be saturated with H₂S by bubbling the gas into the melt using a ceramic tube lance placed just below

the melt line. The processing conditions, time, temperature, and flow rate of H_2S gas will be systematically examined to optimize the incorporation of H_2S into the melt.

Task 4: Glass-Ceraming of Proton Conducting Glasses

Optimized $x\text{H}_2\text{S} + (1-x)\text{B}_2\text{S}_3$ glasses will be processed into glass-ceramic membranes by subjecting the glass to a glass-ceramic processing time-temperature profile. Given the fact that the membrane will operate in a very specific directional manner, that is the protons are expected to conduct across the thin direction of the film, it is important to optimize the underlying ceramic nanostructure and texture to this direction. The preferred texture is to have the microcrystal c-axes aligned in the direction of the preferred conduction.

Subtask 4-1: Proton-doped glassy B_2S_3 samples will be subjected to glass ceraming heat treatments where the glass is heated to a nucleation temperature, held for a period of time, then heated to a slightly higher growth temperature to allow crystalline nuclei to grow and fully crystallize the glass.

Subtask 4-2: Preferred directional growth of the crystallites in the sample will be controlled by inducing nucleation on one side of the sample by quenching one side of the sample. Solidification microstructures will then be encouraged to grow across the thickness of the sample.

Task 5: Characterization of the Physical Properties of Glass Ceramic Proton Conducting Glasses

The fuel cell impedance as a function of temperature and frequency will be measured to determine the proton conductivity as well as the nature of the interfaces between the electrolyte and the electrodes using a Solartron 1260/1296 impedance analyzer. To determine the stability of the GCPCM during operation, cells will be operated at increasing temperatures for increasing periods of time.

Subtask 5-1: The ionic conductivity of the GCPCMs will be determined by using impedance spectroscopy as a function of temperature and frequency.

Subtask 5-2: The electrochemical behavior of the GCPCMs will be determined by using standard cyclic voltammetry methods on GCPCMs configured with platinum electrodes and cycling the electrolyte in voltage between oxidizing and reduction potentials.

Task 6: Characterization of the Structure of GCPCMs

Structural characterization of the GCPCMs will be carried out using IR spectroscopy (examination of the -SH and contaminant -OH structures), Raman spectroscopy (examination of the boron sulfide structures), X-ray diffraction (determination of the crystalline phases formed during glass ceraming), and by ^{11}B and ^1H MASS-NMR (detailed examination of the structure and formation of tetrahedral borons in the glass through the addition of H_2S to the glass). Collaboration with groups in Chemistry (x-ray crystallography) and Physics (NMR) to carry out many of these experiments is necessary.

Subtask 6-1: GCPCMs will be ground together with an excess of IR-grade KBr and pressed into a "KBr" pellet. IR spectroscopy will be used to characterize the relative concentration of -SH (thiol) and -OH (hydroxide) groups in the glass.

Subtask 6-2: Raman spectroscopy will be used to characterize the nature and relative concentration of the boron sulfide structures in the GCPCMs.

Subtask 6-3: X-ray diffraction will be used to determine the relative concentrations and structures of crystalline phases in the material

Design and Development of New Nanoengineering Glass-Ceramic Proton Conducting Membranes (GCPCMs) for High Performance H₂-O₂ Proton Exchange Fuel Cells Iowa State University						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Literature Review						
Review and summarize proton conducting glass-ceramic literature		◆				
Develop literature database			◆			
			◆			
Hiring Research Staff						
Hire post-doctoral research associate, and graduate and undergraduate research assistants	★					
Provide new employee training and orientation		◆				
Synthesis of Proton Conducting Glasses						
Dope glassy B2S3 with protons			◆			
Develop optimized processing conditions			◆			
Glass-Ceraming of Proton Conducting Glasses						
Glass-ceraming of proton-doped B2S3				★		
Preferred directional growth of the glass-ceramic				◆		
Characterization of the GCPCMs						
Measurement of the ionic conductivity					◆	
Electrochemical characterization					★	
Characterization of the Structure of the GCPCMs						
IR spectroscopy					◆	
Raman spectroscopy						◆
NMR spectroscopy						◆
FY 2001 Begins October 1, 2000						

INTERNAL COMBUSTION ENGINES / TURBINES

Internal Combustion Engines Research and Development - Sandia National Laboratories

Internal combustion engine cycles are fundamentally capable of greater than 50% efficiency. In addition, the power output characteristics of an auxiliary power unit (APU) for a hybrid vehicle are different than for conventional cars. By rethinking the problem from a blank sheet of paper a new approach has materialized.

The approach utilizes a free piston oscillating between two combustion chambers, and generating electricity directly from the oscillatory motion of the piston. Combustion occurs when a homogeneous fuel/air charge is compression heated to the point of reaction. In this way both rapid reaction rates, approaching constant volume combustion, and extremely lean mixture combustion, which essentially eliminates NO_x formation, is realized. This appears to be the combustion approach that can achieve both high efficiency and low emissions, but still retain highly developed reciprocating engine technology and fuel flexibility required to transition to a hydrogen energy carrier society.

Since the fuel/air mixture, which is delivered premixed to the cylinder, is ignited by compression heating, the piston position at the time of combustion is determined by compression ratio and initial temperature. The free piston configuration provides a method for controlling the compression ratio electronically, thus allowing continuous optimization of performance and fuel flexibility.

The first goal of their research is to demonstrate the efficiency and emissions performance of a 30 kW generator in a research environment. Following this accomplishment will be refinement of the research unit into a fieldable unit for demonstration, coupled with a wind generator and used for generation when wind power is down.

To date the combustion characteristics of homogeneous charge compression ignition with a free piston have been demonstrated. Also, the design of the linear alternator which converts the piston oscillation to electrical energy is finished. Three alternators from Magnequench International are in house, and the Sandia design alternator parts are fabricated and being assembled. The tasks remaining are the experimental characterization of the linear alternator, design and testing of the two-stroke cycle inlet/exhaust process, development of control system algorithms and hardware, diagnostics and startup processes.

For FY 2001, if funding permits, the following tasks will be accomplished:

Task 1: Fixtures to Mount and Instrument the Linear Alternators and Assemble Prototype

Produce the fixtures required to mount and instrument the linear alternators on the Caterpillar engine for testing. Assemble the prototype for testing on the alternator tester previously developed.

Task 2: Test the Sandia Design Alternator

The alternator by itself will be driven through a 6 inch stroke at 35 Hz by the modified Caterpillar 3304 engine. Measure the electrical output of the alternator and the loads on the stator assembly to determine conversion efficiency. Produce a summary document of the Sandia alternator performance.

Task 3: Test the Magnequench Alternator Design

Produce a summary document of the Magnequench alternator design.

Task 4: KIVA 3V Scavenging Model

Develop with KIVA 3V a scavenging model based on cylinder port (loop) scavenging. Investigate various port configurations.

Task 5: Model Inlet/Exhaust Flow

Model the inlet / exhaust flow of the combustion cylinder utilizing KIVA. Develop a design based on uniflow scavenging.

Task 6: Fabricate Parts

Fabricate the parts for the previously designed scavenging experiment. Demonstrate the performance of the experiment with benchmark testing.

Task 7: Coordinate with CRADA

Share the alternator development data with CRADA partner Caterpillar, in turn receiving piston lubrication, cooling and sealing technology from CAT.

Task 8: NO_x Emission Measurements

Measure the NO_x emissions from the single stroke combustion experiment when operated on ammonia.

Task 9: Modeling and Design

Begin modeling and design of the mathematical engine model and engine starting/control parameters.

Internal Combustion Engines Research and Development Sandia National Laboratories						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Fixture for alternator testing		◆				
Sandia alternator testing report/publication				★		
Magnequench alternator test report						
Loop scavenged design				◆		
Uniflow scavenged design			◆			
Scavenging experiment assembly					◆	
CRADA information exchange					◆	
NO _x emissions from ammonia		◆				
System modeling start			◆			
FY 2001 Begins October 1, 2000						

Reduced Turbine Emissions Using Hydrogen-Enriched Fuels – Sandia National Laboratories

The goal of this program is the development of advanced combustion capabilities for gaseous hydrogen and hydrogen-blended hydrocarbon fuels in gas turbine applications. Driving this interest are several current needs. One need is the cost-effective utilization of alternative fuels with a wide range of heating values. For example, low and medium heating value fuels containing hydrogen are often produced as a by-product in Coal-Gasification Combined Cycle and Fluidized Bed Combustion installations. These product gases could provide a significant source of cost-effective fuels for gas turbines. A second need is related to the recognition that ultra-lean premixed combustion is an effective approach to NO_x emissions reduction from gas turbine engines. Hydrogen blended with traditional hydrocarbon fuels significantly improves flame stability during lean combustion and allows stable combustion at the low temperatures needed to minimize NO_x production. A longer-term need is the desire to minimize and, eventually, eliminate UHC and CO_2 emissions entirely. The use of hydrogen-blended fuels provides both a solution to the immediate need for NO_x reduction, and also provides a transition strategy to a carbon free energy system in the future.

Changes in fuel composition, particularly the addition of hydrogen to hydrocarbon fuels, affect both the chemical and physical processes occurring in flames. These changes affect flame stability, combustor acoustics, pollutant emissions, combustor efficiency and other important quantities. Few of these issues are clearly understood. This program will investigate fundamental issues surrounding hydrogen-enriched hydrocarbon fuel use and will include fundamental studies of chemical kinetics, combustion fluid dynamics, laminar and turbulent flame structure to better define and understand these issues.

The initial phase of this program will be carried out at atmospheric pressure, in laboratory-scale combustor configurations representative of gas turbines. Laser diagnostics developed at the Sandia Combustion Research Facility will be applied to the study. These diagnostics include Planar Laser-Induced Fluorescence (PLIF) from OH which provides data on the instantaneous flame zone structure, particle image velocimetry, which measures the instantaneous velocity and strain field, and laser-Doppler velocimetry which measures the three-component velocity statistics. PLIF from acetone seeded into the fuel will be used to characterize the mixing process. The experimental work will be closely coupled with numerical modeling efforts to provide the fundamental data needed for model validation and development.

During the coming year the experimental program will utilize two burners being developed in collaboration with NETL and NASA. These collaborations allow us to leverage existing, internally-funded programs at NETL and NASA and provide access to laboratory facilities that allow testing at the high pressures and temperatures typical of gas turbine operation. The first burner, being developed in collaboration with NETL, is a lean premixed swirl-stabilized burner representative of power-generation gas turbine combustors. The burner was designed to provide well-defined inlet and boundary conditions to facilitate the development of a database for model validation. During next year, a range of hydrogen/natural gas blends will be studied to quantify the effect of hydrogen addition on lean flame stability and on the extension of the lean flammability limits to minimize NO_x production. Activities at Sandia will include atmospheric investigation of combustion fluid dynamics and flame stability, development of diagnostics for turbine combustion, and fundamental model development of relevant flows. In particular, the effects of hydrogen addition on lean burner operation will be quantified. Activities at NETL will include investigation of combustion fluid dynamics and stability at elevated pressure and temperature and model development for high pressure, high inlet temperature flows.

The burner being developed with the NASA Glenn Research Center focuses on the use of hydrogen as an alternative aircraft fuel and is part of the NASA Zero CO₂ Emissions Technology Program. Sandia will apply laser-based diagnostics to characterize flames in a fuel nozzle designed for use with premixed hydrogen and air. The work will explore fundamental issues associated with flame stability, flashback, pollutant emissions, turbulent mixing and flame structure. The first generation nozzle effectiveness will be evaluated and modifications implemented to improve performance. Work at NASA Glen will focus on full-scale nozzle configurations operating at high-pressure conditions typical of aircraft gas turbine operation.

**Reduced Turbine Emissions Program
Sandia National Laboratories**

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Lean-Premixed Swirl Burner						
Design and fabricate burner	◆					
Characterize burner options		◆				
Quantify effect of hydrogen addition on flame stability		★				
Complete OH PLIF measurements			◆			
Complete velocity measurements				◆		
Hydrogen Burner						
Design and fabricate burner	◆					
Characterize burner operation		◆				
Evaluate fuel/air mixing and implement improvements			◆			
Complete OH PLIF measurements					◆	
Complete velocity measurements						◆

FY 2001 Begins October 1, 2000

Hydrogen / Natural Gas Blends – NRG Technologies

NRG Technologies, Inc. is developing a critical database and hardware implementation of the addition of hydrogen to natural gas to produce ultra-low exhaust emissions of controlled pollutants for applications now using diesel engines. The project will conduct research in spark-ignited internal combustion engines for extremely high values of BMEP (>1.4 MPa). In addition, these research results will be used to configure candidate hardware configurations that can successfully utilize fuels consisting of mixtures of hydrogen and natural gas. The design objective being to produce a viable configuration that can replace existing diesel engines with hydrogen-enriched natural gas (HCNG).

Producing ultra-low amounts of harmful exhaust emissions from heavy-duty vehicles requires a markedly different strategy from reducing emissions in light-duty vehicles, largely due to the relative power-to-weight ratios for the two types of vehicles. Light-duty engines typically produce much more ultimate power than is required by the emissions certification driving test. In contrast, heavy-duty engines are typically used at their maximum power a great deal of the time, and the heavy-duty emissions test mirrors that use. This difference becomes significant when charge dilution is used as a NO_x control strategy.

Task 1: Examine the Effects of Compression Ratio

Because HCNG has a high octane rating it is capable of being viable at much higher compression ratios than the 12-1 tested previously. Compression ratios up to 15-1 will be tested and evaluated for tradeoffs of efficiency, power output, and emissions levels.

Task 2: Examine the Effects of Ignition System Types

One of the major answers desired from this subtask is to determine the relationship between number of spark plugs, the location of the spark plugs, and the ignition energy associated with each spark event.

Task 3: Examine the Effects of EGR-to-Lean Burn Ratio

For heavy duty engines, the engine efficiency is considerably more important than it is for light duty engines. Under the high BMEP conditions investigated, maps will be created to compare A equivalent at equivalence ratio vs. exhaust emissions for various combinations of EGR and lean burn. These combinations will also be evaluated for tradeoffs of efficiency, power output, and emissions levels.

Hydrogen/Natural Gas Blends NRG Technologies						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Cylinder head investigation	◆					
Compression ratio investigation		◆				
Ignition system investigation			◆			
ERG-to-lean burn investigation				◆		
Exhaust catalyst investigation					◆	
Water injection investigation						◆
Final engine design parameters						★
FY 2001 Begins October 1, 2000						

Task 4: Examine the Effects of Exhaust Catalysts

A number of single brick oxidizing catalyst systems from several automotive catalyst manufacturers will be evaluated. The critical reaction component for these tests will be ethane emissions. Emissions testing will be conducted at both high and low BMEP conditions due to the strong exhaust gas temperature dependence on engine load.

HYDROGEN SAFETY

Interfacial Stability of Thin Film Hydrogen Sensors – National Renewable Energy Laboratory

The real and perceived hazards of hydrogen fuel use, its production, and storage require extensive safety precautions and codes to be put in place before any serious movement can be made towards a hydrogen based energy future. Currently, commercial hydrogen detectors are not useful for widespread use, particularly in transportation, because they are too bulky, expensive, and dangerous. Recent work sponsored by the DOE Hydrogen Program has developed promising technologies for satisfying the future demands. Sensors that exhibit physical or optical changes when exposed to hydrogen have been fabricated and tested, and promise to provide inexpensive hydrogen detection. For example, there are thick film and thin film metallic sensors that exhibit conductivity changes when hydrogen adsorbs on the surface and is incorporated into the lattice. There are thin film sensors that are deposited as a part of a field-effect transistor, where accumulation of atomic hydrogen at the metal/insulator interface results in a change of response from the circuit. Finally, there are chemochromic sensors, where reaction of thin films with hydrogen gas results in an optical change that can be sensed by a probe beam of light. All of these sensors have the potential for degradation in their performance over time due either to mechanisms that are inherent in their construction, a result of their cyclic interaction with hydrogen, or contamination from impurities in the environments in which they will be used. Prior research to study those issues has ranked their importance to the various sensor concepts, has at least suggested the relevant mechanisms, which has pointed to methods which may mitigate these factors. The research outlined here addresses those issues and will be directed toward substantially extending the lifetime and utility of these sensors.

The goals of this project are to better understand the mechanisms that contribute to long term loss of performance in low cost hydrogen sensors. NREL will explore methods (suggested by this developing understanding) for increasing the durability and reliability of these sensors.

Study of failure mechanisms in optical hydrogen sensors has indicated that there are distinct modes for different types of sensors. The two types of sensors studied were those using metal oxides as the optically active layer and those using metal hydrides. Each type of sensor is discussed in turn.

Metal hydride sensors use (typically) rare earth hydrides as the active layer with a palladium overlayer to function as a hydrogen dissociation catalyst. The rare earth hydrides are characterized by the ability to react with atomic hydrogen to form distinct metal hydride compounds with various oxidation states. For instance, GdH_2 can be used as the active optical layer of a sensor. When exposed to a sufficient concentration of atomic hydrogen, it reacts (more or less) reversibly to form GdH_3 . The two compounds have significantly different electronic properties that manifest themselves at optical wavelengths. GdH_2 is conductive and highly reflective in the visible. GdH_3 is a poor conductor and is transparent in the visible. When hydrogen is removed from the proximity of the sensor, GdH_3 decomposes spontaneously to GdH_2 . Hence, a measure of the reflectance of a light beam off the composite film layer can be used to produce a signal that indicates the presence or absence of hydrogen. However, extensive analytical investigations showed that cyclic exposure to hydrogen, particularly at concentrations greater than 2%, caused cracking in the composite film structure followed by delamination from the substrate materials (glass and acrylic). In this degradation mode, 1 to 20 exposures were sufficient to cause significant degradation in the signal response. This degradation was not reversible and was irreproducible from sensor to sensor.

There is also a degradation mode related to reversible and irreversible reactions in the palladium dissociation catalyst. A clean Pd film exposed to contaminants in the air such as CO , CH_4 , and H_2S will

become contaminated and lose its ability to dissociate hydrogen. This greatly affects the rate of response of the sensor, or, in the case of H_2S , can completely kill the response of the sensor. This loss of performance takes place from days to weeks in ambient air, depending upon the concentration of contaminants in that air. This mode of degradation is common to all sensor types using palladium as a hydrogen dissociation catalyst.

Another degradation mode has been recognized in some of the optical sensors. Variations in the charge transfer across the interface affects the rate of proton diffusion into the optically active layer. The microscopic details of the electronic properties of the materials at the interface control this transfer and, thus, the optical response of the sensor. There appear to be either physical or chemical (or both) changes in these interfacial properties after many cyclic hydrogen insertion reactions. It is important to understand why these changes occur and how to slow or prevent them. NREL feels that it is likely that very subtle changes in the interface structure and/or the insertion of dopants can control the response of these interfacial properties.

Finally, a mode of degradation has been recognized that is a result of changes in the bulk properties of the active, metal oxide layer. The ability of the material to diffuse and react with hydrogen is affected by both its bulk structural configuration and by its chemistry. For instance, a very small loss in oxygen concentration in the metal oxide can change this material from one that shows an excellent coloration response to hydrogen to one that responds only to the first application of hydrogen, then reacts no further. Water of hydration is important for some of the MO_x films, and this must be rigidly controlled to produce films of acceptable response. Additionally, the porosity of the layer plays a roll in the diffusion rate of hydrogen into and out of the material. NREL finds that very small changes in deposition conditions can elicit huge changes in the response of the material to hydrogen. All of these factors need to be understood and controlled. Control can likely come from selecting exactly the correct deposition conditions and, perhaps, by doping the material to control its chemical potential with respect to hydrogen.

Research work this year will address the issues identified in FY 2000. Fouling of the dissociation catalyst is a very important issue, because this affects every sensor type. NREL believes that they have already discovered means of mitigating the issue of structural changes in the Pd, due to cyclic exposure of the catalyst to hydrogen and exposure to concentrations of hydrogen in excess of 2%. Therefore, minimal activity in this area is planned this year. Effort will be allocated to understanding and controlling the Pd/ MO_x interface and to understand the effects that alteration of the structure and chemical potential of the MO_x has on the performance and lifetime of the sensor.

Task 1: Pd Surface Stabilization

NREL will pursue two avenues for altering the Pd surface to mitigate the effects of fouling of the catalyst over time. One will be to use mixed phase alloy materials that can act as surface scavengers. These will produce islands of material on the surface that will react with the contaminant molecules more strongly than the palladium. The second avenue will use unique surface coatings that can selectively hinder access of the contaminant molecules to the Pd surface. They already have strong indications that such coatings can greatly increase the surface resistance to fouling.

Task 2: Study the Pd/ MO_x Interface

NREL will fabricate special test articles that will allow them to study the interface of these materials with electrochemical impedance spectroscopy (ECIS). The basic setup for ECIS is already resident within NREL laboratories, but they will fabricate a test chamber that will allow them to study the complex

impedance of the interface as a function of the temperature and partial pressure of a mixed gas stream flowing over the test article.

Interfacial Stability of Thin Film Hydrogen Sensors National Renewable Energy Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Pd Surface Stabilization						
Report progress on stabilizing the Pd surface to contaminants					★	
Study the Pd/MO_x Interface						
Design and construct test chamber for conducting impedance spectroscopy in controlled environments				◆		
FY 2001 Begins October 1, 2001						

Integrated Micro-Machined Hydrogen Gas Sensor - Advanced Technology Materials, Inc.

The U.S. Department of Energy has been mandated to develop the technologies required for the implementation of hydrogen energy, which includes production, storage, transport, and utilization. A common need to each of the areas is the ability to detect and monitor gaseous hydrogen. This is critical not only for health and human safety, but also for the development of highly efficient hydrogen processes. Hydrogen gas sensors that can quickly and reliably detect hydrogen over a wide range of conditions and concentrations are not currently available, and must be developed to facilitate the transition to a hydrogen based energy economy.

Advanced Technology Materials, Inc (ATMI) approach to meet these required hydrogen detection needs is the development of MEMS (Micro-Electro-Mechanic System) based, solid-state, hydrogen gas sensors. These sensors couple novel thin films as the active layer on device structures known as micro-hotplates. This coupling has resulted in a gas sensor with several unique advantages in terms of speed, sensitivity, stability, power consumption and amenability to large scale manufacture. To date, ATMI has demonstrated speeds of response of less than 0.5 seconds, and levels of response of greater than 120% to H₂ concentrations of 0.25%.

Task 1: Sensor Design and Fabrication

ATMI will continue to build on the work of year one, and concentrate on the optimization of device design as well of the device processing. In the design optimization, they will minimize the device size and power requirements, while process optimization will concentrate on maximizing device yield. Each optimization will also use feedback from the sensor response testing in the following tasks.

Task 2: Short Term Response Testing

ATMI will continue to use the automated gas sensing manifold developed last year to test for the effect of potential contaminant gases on sensor performance. In addition, the effort to examine cross sensitivities and contaminant gases, as well as temperature effects, will be expanded through a collaboration with an outside partner.

Integrated Micro-Machined Hydrogen Gas Sensor ATMI, Inc.						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Sensor Design and Fabrication						
Choose best MEMS design			◆			
Optimize functionalization process					◆	
Short Term Sensor Testing						
Complete contamination testing ATMI			◆			
Complete cross-sensitivity testing collaborator						◆
Long Term Sensor Testing						
Determine drift mechanism				◆		
Demonstrate extrapolated life time						★
FY 2001 Begins October 1, 2000						

Task 3: Long Term Behavior Investigation

The long term stability and behavior of the sensor is an important consideration for most potential applications. ATMI will perform experiments to develop an understanding of potential drift mechanisms of these devices and the effect operating conditions have on these mechanisms. This task will tie in closely with the tasks above, and the ultimate goal of this will be to demonstrate an extrapolated lifetime of 3 years.

Codes and Standards Analysis – University of Miami

This project builds on previous safety analyses of hydrogen conducted at the University of Miami. In particular, the hydrogen risk assessment method used previously to predict the motion of leaking hydrogen clouds. It has been shown that the accumulation of hydrogen, leaking into an enclosure, can be accurately predicted with a helium verified CFD model. The computer model verification demonstrates the ability of the model to accurately predict the behavior of helium in the geometry of concern. The verified CFD model is then used to analyze the behavior of hydrogen. The accumulated concentration of hydrogen, predicted by the model, can be used to predict the likelihood of accidental ignition. It has been shown that helium behaves very similarly to hydrogen when leaked into an enclosure.

A hydrogen risk assessment method has been under development for the last four years at University of Miami. A two-year work effort, applying the method to the design of garage doors, was funded by Ford Motor Co. through DTI from 7/96 through 5/98. The proposed work may produce further simplifications of the existing method for the case when only the path of leaking hydrogen is needed.

Task 1: CFD Model - California Fuel Cell Building

This task involves the creation of a CFD model of California Fuel Cell Building in Sacramento. Once the model is created it will be run three times (Part A-2). Because the model will be large it is anticipated that no more than three runs should be conducted. The first two runs will be used to show the effects of vehicle location. The third run will be used to further show the effects of vehicle location or to show the effects of bulk airflow, whichever is deemed most informative.

Task 2: CFD Model - Warehouse

Subtask 2-1: Is the creation of a CFD model of a 5,000 square foot warehouse with an 18-foot ceiling. The warehouse, in which the ongoing hydrogen safety analysis is being conducted, has these dimensions. It also contains four independent air conditioning systems that can produce a variety of circulation patterns in the fully air conditioned building. Tests will be made with leaking helium and hydrogen at low leakage rates to validate the model's ability to predict hydrogen gas motion from helium gas motion. Then tests will be made with helium to allow a verified prediction hydrogen gas motion. This is an application of the "Hydrogen Risk Assessment Method" developed and published during ongoing and previous research.

Subtask 2-2: Will use the model to predict the gas motion created by high leakage rates of hydrogen.

Subtask 2-3: Will develop an apparatus and procedure that creates helium bubbles of the proper size and density to approximate the path of leaking hydrogen. It is felt that this will be possible because even though hydrogen and helium differ in density, they still transverse similar paths when released in an air environment. The buoyancy forces that dominate the flow are similar, though helium is twice the density of hydrogen, because both densities are so much lower than the density of air. The size and degree to which released soap bubbles are connected to one another can be controlled with the geometry of the holes creating the bubbles.

Task 3: Home Refueling System Survey

Subtask 3-1: Survey of potential home refueling systems. A number of projects are presently directed at providing home refueling systems for hydrogen fueled vehicles. The flow rate at which these systems

might leak hydrogen and the total volume of hydrogen they could leak are a function of the design of the system.

Subtask 3-2: The purpose of the survey is to gather information needed to determine how much, and at what rate, the various systems may leak hydrogen.

Subtask 3-3: The University of Miami has previously modeled hydrogen leakage in garages for DOE and Ford Motor Company. The same single car residential garage model will be used for modeling the effects of hydrogen leakage from a home refueling system.

These three tasks are the three tasks presented at the Annual Review. Task 1 has been modified by including the site selected by DOE headquarters.

Codes and Standards Analysis University of Miami						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Create model of California Fuel Cell Building in Sacramento		◆				
Model leakage at 3 car locations or 2 car locations and 1 ASHRAE noncompliance scenario				★		
Create experimentally verified model of 5000 sqft building			◆			
Model hydrogen releases in building			◆			
Develop helium bubble procedure to duplicate hydrogen motion				★		
Survey home refueling systems	◆					
Determine potential leakage rates and release volumes			◆			
Model leaks in residential garage				★		
Final write-ups						◆
FY 2001 Begins October 1, 2000						

Hydrogen Infrastructure Activities – National Renewable Energy Laboratory

In October 1999, the U.S. Department of Energy (DOE), the California Air Resources Board (CARB), and the California Energy Commission (CEC) co-sponsored a workshop to answer the question: ***What has to be done, beginning today, to implement a hydrogen fuel infrastructure so that when hydrogen vehicles become market-ready in 3-5 years, the infrastructure needed for on-board direct use of hydrogen will be available?*** As a result of the workshop, the ***Blueprint*** for Hydrogen Fuel Infrastructure Development was formulated.

An additional focus of this project is to assist DOE in fostering the development of Codes and Standards (C&S) for hydrogen applications by playing an active role with C&S organizations. In addition, efforts will also be geared towards incorporating hydrogen safety issues into existing and proposed national and international codes.

The goal of the ***Blueprint*** is to outline a five-year action plan to develop a hydrogen fuel infrastructure needed by the 2003 - 2004 timeframe for both heavy-duty and light-duty vehicles. The ***Blueprint*** is based on a consensus among the workshop participants on the desirable attributes of a hydrogen fuel infrastructure, as well as on an estimate of the number, type, and uses of hydrogen vehicles anticipated in the 2000-2005 time. The ***Blueprint*** also explores how addressing near term requirements and barriers will facilitate establishment of a commercial-scale hydrogen fuel infrastructure.

The goal of the C&S effort is to facilitate market acceptance and deployment of hydrogen. The focus is on the Transportation sector (using hydrogen fuel cells and internal combustion engines) and the Buildings sector (using fuel cells). For these applications, the C&S work will cover producing, transporting, storing, dispensing and utilization of hydrogen in fuel cells and internal combustion engines.

Subsequent to the October 1999 workshop, the ***Blueprint*** Core Team met on February 29, 2000, and May 8, 2000. The Core Team has membership from Ford Motor Company, California Energy Commission, Shell Hydrogen, Stuart Energy Systems, and Praxair, Inc. Technical support is provided by NREL and SNL. A third meeting was held September 21-22, 2000, in Las Vegas, Nevada. The purpose of the meeting was to convene a roadmapping session to support the development of a five-year action plan. The four focus areas for the roadmapping efforts include: (1) standardized dispensing station design; (2) test and certify hydrogen containers; (3) integrated codes and standards; (4) safety RD&D for public use of hydrogen.

In April 2000, the International Codes Council (ICC) Board of Directors approved the appointment of an Ad Hoc Committee to address the subject of hydrogen used in fuel cells in vehicular or portable applications. The ICC concluded that the subject of stationary fuel cell power plants is already being well addressed in the International Codes. The ICC Board established a nine-member Ad Hoc Committee consisting of three code officials, three industry representatives and three design professionals. It held its first meeting on August 29-30, 2000. NREL participates as an ex officio member.

In May 2000, the National Fire Protection Association (NFPA) published NFPA 853 "Standard for the Installation of Stationary Fuel Cell Power Plants." It covers consensus standards for the design, construction and installation of stationary fuel cell power plants with a gross electric power of at least 50 kW. In addition, NFPA's Standards Council formally approved the establishment of a project to develop a building code – NFPA 5000. This effort, which is just starting, will include hydrogen fuel systems. Mr. Algis Vasys of Cambridge Associates (under subcontract to NREL) has been nominated by DOE/HQ to

participate in this activity. The NFPA also announced in FY 2000 that it will develop its own building code standards relating to hydrogen.

Task 1: Blueprint for Hydrogen Infrastructure

Based on the results from the September 21-22, 2000 meeting, detailed action plans will be developed for each of the four focus areas mentioned above. In some cases, additional information will be solicited from the hydrogen community via a Hydrogen Program solicitation.

Collaborative efforts will include inputs from the California Fuel Cell Project, the hydrogen bus demonstration projects, and the Fuels for Fuel Cells effort underway in the DOE Office of Transportation Technologies.

Task 2: Codes and Standards Support

Subtask 2-1: Building Code and Fire Safety Codes Officials Familiarization and Marketing Research

NREL will work with DOE to: (a) familiarize building code and fire safety officials in strategic states and communities with hydrogen for transportation and buildings applications; (b) determine the most critical, near-term codes and standards needs (from the perspective of building code and fire safety officials); and (c) determine, through a systematic marketing research effort involving focus group sessions, the particular issues and concerns pertaining to hydrogen use.

Subtask 2-2: Comprehensive Hydrogen Safety Code Development

The activities of this task will: (a) support and facilitate the development of national and international codes and standards by the ICC, BOCA and NFPA; and (b) report on the status (annually) of the development of standards and barriers to their development. NREL will assist Program interactions with both ICC and NFPA with respect to the development of codes and standards. In addition, as applicable, NREL will support BOCA and other entities in codes and standards development. An annual status report on hydrogen codes and standards will be generated and delivered at the NHA and HTAP conferences each spring.

Hydrogen Infrastructure Activities National Renewable Energy Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Blueprint for Hydrogen Infrastructure						
Solicitation posted on website		◆				
Selection of awards			★			
Contract monitoring					◆	
Codes and Standards Support						
Draft of brochure			◆			
Participate in ICC meetings					◆	
FY 2001 Begins October 1, 2000						

High Efficiency Steam Electrolyzer – Lawrence Livermore National Laboratory

The objective of this project is to develop a novel, low cost and highly efficient high temperature steam electrolyzer for distributed hydrogen production. Although water or steam electrolysis is well known to be one of the cleanest ways to produce hydrogen, wide spread utilization is hindered by high operational cost due to high electricity consumption. LLNLs approach to decrease the electricity consumption in electrolysis is to use natural gas as an anode depolarizer. This approach replaces one unit of electricity by one equivalent energy unit of natural gas at one-fourth the cost. There are two possible modes of operation. In the total oxidation mode, i.e. when methane is used only for the purpose of reducing the chemical potential difference between the two sides of the electrolyzer membrane, the system does not require any gas separation and has the potential to produce pure hydrogen at high pressure. In the partial oxidation mode, methane is converted to hydrogen and carbon monoxide, which is subsequently converted to hydrogen via the water gas shift reaction. LLNL chose to focus their current efforts on the development of a system operating in the total oxidation mode because of its simplicity. Using the appropriate system design, it is possible to electrochemically compress hydrogen in-situ, thus eliminating the need for an expensive hydrogen compressor.

LLNL is also considering additional advanced modes of operation for the electrolyzer. Using appropriate materials, the electrolyzer can be made to operate in the fuel cell mode to generate electricity from natural gas. The ultimate device will be a highly flexible system that can produce hydrogen fuel for transportation and electricity for power.

The goal for FY01 will be the development of a second-generation electrolyzer stack producing 200 W equivalent of hydrogen and operating at 150 psi.

Task 1: Optimize Single Tube

This task will include efforts being focused on the anode composition and microstructure for better oxidation of methane. Tube extrusion will also be developed to substitute for the cold isostatic press approach that LLNL are currently using. The extrusion process is more suitable for mass production of ceramic tubes. In preparation for high pressure operation, fabricated tubes will be tested under a high-pressure gradient to evaluate their mechanical integrity.

Task 2: Demonstrate Bimodal Operation-Production of Hydrogen or Electricity Using the Same Cell

In FY00 LLNL showed that it is possible to use the same electrolyzer system to produce both hydrogen and electricity. This dual production requires an electrode material that is stable in both reducing and oxidizing atmospheres. LLNL will investigate different electrode materials to optimize this material. Performance in both electrolysis and fuel cell modes will be characterized. The constraints on the system design will be identified.

Task 3: Develop Second Generation Electrolyzer Stack

Several different brazing and soldering techniques will be evaluated to make a gas-tight seal between the electrolyzer tubes and the stainless steel tubing of the gas manifold system. This task will also look to increase the electrolyzer electrical efficiency. A simple tube-to-tube connection using copper fittings will be developed. A 200 W system will be also be fabricated for test.

Task 4: Demonstrate a 200 W Electrolyzer Stack Operating at 150 psi

The system will be characterized at atmospheric pressure as well as at 150 psi. The effect of pressure on the system operation will be investigated.

Task 5: Complete System Analysis

This analysis will allow them to evaluate and optimize system performance necessary to ultimately reach the desired goal of a system with kW capacity.

High Efficiency Steam Electrolyzer Lawrence Livermore National Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Optimize Single Tube						
Optimize component materials for better kinetics	◆					
Optimize tube fabrication process using extrusion			◆			
Complete characterization of single tube under pressure			◆			
Demonstrate Bimodal Operation-Production of Hydrogen or Electricity Using the Same Cell						
Electrode materials optimized for bimodal operation			◆			
Performance in both fuel cell and electrolyzer modes characterized				◆		
Develop Second Generation Electrolyzer Stack						
Develop a metal-to-ceramic seal to make gas tight			◆			
Develop a tube-to-tube series connection for increased efficiency			◆			
Complete stack construction of a 200 W system				◆		
Demonstrate a 200 W Electrolyzer Stack						
System will be characterized at ambient and 150 psi					★	
Complete System Analysis						
System analysis done to optimize performance						◆

FY 2001 Begins October 1, 2000

3.2 Technology Validation

This section describes the projects that are being considered as key hydrogen implementation components. They include projects pertaining to renewable hydrogen systems, projects that will lead to the development of a hydrogen infrastructure, and projects that will lead to the development of hydrogen in remote areas. Technology Validation Tasks are listed in Table 3.5.

Table 3.5 Technology Validation		
Goal: Support industry in the development and demonstration of hydrogen systems in the utility and transportation sectors		
Category	Project	Researcher
<i>Renewable Hydrogen Systems</i>	Engineering Scale Up of Renewable Hydrogen Production by Catalytic Steam Reforming of Peanut Shells Pyrolysis Products	National Renewable Energy Laboratory
	Hydrogen Production Through Electrolysis	Proton Energy Systems
	Renewable Hydrogen System Integration and Performance Modeling	Desert Research Institute
	An Integrated PV / Electrolysis / Metal Hydride Hydrogen Generation and Storage System for Scooter Applications	Energy Conversion Devices, Inc.
	Hydrogen-Based Utility Energy Storage System	SRT Group
<i>Hydrogen Infrastructure</i>	Filling up With Hydrogen 2000	Stuart Energy Systems
	Light, Medium Duty Fleet	NRG Technologies
	Hydrogen Commercialization for the 21 st Century	SunLine Services Group
	Hydrogen Reformer, Fuel Cell Power Plant and Vehicle Refueling System	Air Products and Chemicals, Inc.
	Hydrogen Composite Tank Program	IMPCO
	OTT Solicitations	TBD
	Insulated Pressure Vessels for Vehicular Hydrogen Storage	Lawrence Livermore National Laboratory
	Refueling Infrastructure for Fuel Cell Underground Vehicles Including a Locomotive	TBD
<i>Remote Power</i>	Alaska PEM Fuel Cell Validation Project	University of Alaska, Fairbanks
	Power Parks System Simulation Project	Sandia National Laboratories
	Alaskan PEM Fuel Cell Validation Projects	Sandia National Laboratories

RENEWABLE HYDROGEN SYSTEMS

Engineering Scale Up of Renewable Hydrogen Production by Catalytic Steam Reforming of Peanut Shells Pyrolysis Products – National Renewable Energy Laboratory

By integrating hydrogen production with existing industrial utilization of agricultural residues, economic barriers can be overcome in the near-term time frame so that hydrogen may be produced at a cost similar to that from existing hydrocarbon-based reforming technologies. NREL will assist a team of industrial and academic organizations from Georgia who are adapting NREL's steam reforming process to an existing process for making activated carbon from densified peanut shells. This integrated strategy will substantially demonstrate the potential impact of hydrogen and bioenergy on the economic development and diversification of rural areas. The hydrogen produced will be blended with CNG and used to power a bus in the near by city of Albany, GA. This demonstration will facilitate the local use of hydrogen and prepare the basic infrastructure for large-scale production and use in the three-year time frame.

The goals and objectives of the project are:

- To assist Clark Atlanta University and Scientific Carbons Inc. in the design of the 10-20 kg/hour fluid bed catalytic steam reformer system.
- To conduct the system shakedown at NREL by interfacing with the Thermochemical Users Facility (TCUF). NREL's experience with the development of the technology and the available analytical capabilities of TCUF will allow the reactor to be characterized and optimized for the subsequent operation on a slipstream of the Scientific Carbons pyrolysis products.
- To participate in the design of the process modifications that will be necessary to integrate the reactor safely and efficiently in the existing Scientific Carbons process.
- To support the partnership development that will be necessary for the bus demonstration.
- To identify, with the Georgia Institute of Technology, other biomass resources in the region that could be used to produce hydrogen in conjunction with the Scientific Carbons process or by other integrated biomaterial processing technologies.

During FY 2001, this technology validation project will focus on reactor scale-up, with supporting activities to prepare for subsequent commercialization of the process in a three-year time frame. The primary focus is to undertake process validation studies for the use of peanut shells produced in Georgia as feedstock for the pyrolysis-steam reforming process. The process combines two stages: slow pyrolysis of biomass to generate charcoal; and catalytic steam reforming of the pyrolysis vapors to hydrogen and carbon dioxide.

Phase 1, to be performed in FY 2001, focuses on development of an engineering scale system to validate the concept of catalytic steam reforming at an appropriate scale. NREL will provide data on the previous bench scale studies and technological know-how on the fast pyrolysis and catalytic steam reforming, for application to the slow pyrolysis process. Scientific Carbons Inc is currently operating a pilot facility in Blakely, GA to convert 1000 kg/hr of pelletized peanut shells to activated carbon. Scientific Carbons' facility can be used to perform a scaled-up demonstration of a steam reforming process to convert the off-gas of the peanut-shell carbonization process to hydrogen. As a small company with a demonstrated ability to build modular systems, their current process could be modified and expanded to run a variety of other feedstocks and to make a range of alternative products.

Task 1: Design and Construction of Catalytic Fluid Bed Steam Reforming Reactor

NREL staff will support the detailed design and construction activities of the engineers at Clark Atlanta University and Scientific Carbons who will be designing and building the 10-20 kg/hour (of pyrolysis vapors) system. NREL's expertise and experience over the last two years in running the bench scale unit are essential to this effort. In addition, the unit will be designed and operated with the NREL Thermochemical Users Facility (TCUF) pyrolysis unit, in addition to a slipstream of the Scientific Carbons' process stream.

Task 2: Installation and Shakedown of the Reactor at NREL

The reactor will be installed at NREL and is expected to take two months. The initial shakedown of the reactor will be performed at the TCUF. Bench-scale research has occurred at this facility for over 4 years. By performing the initial system tests at NREL, the expertise of those researchers and the state-of-the-art analytical equipment of TCUF can be used to monitor and adjust/optimize the system performance. A 10-20-kg/hr fluid bed pyrolysis unit at TCUF will be able to feed the steam reforming unit for the shakedown.

The catalyst, in a form suitable for fluid bed, is not commercially available and hence will be commissioned from S&D-Chemie (formerly United Catalysts). Initial tests will monitor catalyst fluidization and attrition under simulated conditions. Methane reforming will be used to verify catalyst performance. Subsequent runs with pyrolysis vapors will be performed until performance matches previous work at the bench scale.

Task 3: Preparation for Installation at the Scientific Carbons Site

NREL will support the work performed by Scientific Carbons and Clark Atlanta University on the preparation for the testing that will occur in the second year at the industrial site. This will include an assessment of the impact of the long-term steam reforming tests on the mass and energy balance of the current Scientific Carbons operation. The existing pyrolysis facility owned and operated by Scientific Carbons, will be modified as follows:

- Design, construction and addition of a slip stream capable of withdrawing 10-20 kg/h of pyrolysis vapors
- Installation of instrumentation and on-line monitoring and data acquisition for the above system for product stream analysis, and process mass and energy balance.

Task 4: Cost Analysis for Hydrogen Production from Alternative Biomass Feedstocks

Feedstock issues, such as supply, cost, logistics and the value of co-products, will be a major factor in cost-effectiveness of the hydrogen production process. In this task, NREL will support Georgia Tech's work to develop decision models for selecting among feedstock, process, and deployment alternatives. Of particular interest are peanut shells supply and cost projections and the evaluation of other agricultural residue feedstocks available in the same geographical area. Process economics will be developed for the major process options and used to construct a process options database. Different network options will be developed to determine optimum subdivision of tasks among potential sites and to develop criteria for location of new processing sites. The evaluation of other co-products will also be included.

**Engineering Scale Up of Renewable Hydrogen Production by Catalytic Steam Reforming of Peanut Shells
Pyrolysis Products
National Renewable Energy Laboratory**

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Design and Construction of Catalytic Fluid Bed Stream Reforming Reactor						
Design and construction of fluidized bed reformer				★		
Installation and Shakedown of the Reactor at NREL						
Complete shakedown					◆	
Preparation for Installation at the Scientific Carbons Site						
Complete design of steam reforming system interface for the Scientific Carbons site						◆
				◆		
Cost Analysis for Hydrogen Production from Alternative Biomass Feedstocks						
Report					◆	

FY 2001 Begins October 1, 2000

Hydrogen Production Through Electrolysis - PROTON Energy Systems

In PROTON's original proposal, work in Phase II was to focus on demonstrating PROTON's UNIGEN[®] regenerative fuel cell technology. This technology, once matured, will enable PROTON[®] electrolyzer hardware to work in both directions—as both an electrolyzer making hydrogen and as a fuel cell converting that hydrogen back into electricity. There are many advantages of an integrated unit that makes hydrogen, stores it at pressure and then reverses the flow to make power as needed.

As PROTON looked at what they learned during the Phase I activity and how to proceed to the Phase II it was clear to them that the electrolyzer is the key to a successful deployment. As the future unfolds, regardless of which renewable technology provides the electricity to make the hydrogen or which technology converts the hydrogen back into electricity, all require that the electrolyzer be reliable and inexpensive. Numerous companies are currently at work on the various methods of renewable electricity (e.g. Dish/Stirling, PV, Wind) and energy conversion (e.g. fuel cells, engines), but few companies are working on the most difficult and most critical link to a fully integrated renewable system, the electrolysis system.

PROTON proposes to reduce the cost of their hydrogen generator family by 50% in the next two years and show evidence of further dramatic reductions in the years beyond. They will do this by focusing cost reduction efforts on three key elements of the electrolyzer, the electrolysis cell stack, the power conditioning and renewables interface, and the electrical controls and software. PROTON will implement these reductions on their smaller (HOGEN[®] 40) electrolyzer first and expand those improvements to the larger electrolyzer towards the end of the program. All of the improvements undertaken on this program will benefit the full line of electrolyzers so that the cost to large and small energy storage applications will be reduced. They propose to build a HOGEN 40 within the first twelve months of the program that implements all or most of the improvements undertaken. In addition, they will subsequently modify one or more HOGEN 300/380 systems by the end of Phase II to prove out the cost reductions in the large sized generator.

Task 2: Cell Stack Cost Reduction

Subtask 2-1: Support components

The electrolysis cell stack has traditionally used machined endplates and a spring washer configuration on tie rods to maintain proper mechanical compression on the individual cell components. Work will be done to redesign the endplates for implementation of a near-net-shape process such as casting or powder metallurgy that minimizes the amount of material that is used and further reduces process time.

Subtask 2-2: Membrane and electrode

The goal of this task is to optimize the membrane and electrode assembly. This will include optimization of the amount of catalyst applied to both the hydrogen and oxygen sides of the electrode as well as the method of those applications. Techniques for catalyst application that will be investigated will include certain approaches utilized in the manufacture of fuel cell MEA's such as silk screening of inks and application of dry powders. State-of-the-art electrolyzer oxygen electrodes that are generally proprietary precious metal formulations will be used instead of typical fuel cell grade platinum/carbon materials.

Subtask 2-3: Flow fields

The goal of this task is to develop a lower cost electrode support material and implement advanced configurations conceived by PROTON. This involves the characterization of materials that are

electrically conductive, corrosion resistant, mechanically robust, and offer the proper fluids carrying capability required for high performance

Task 3: Power Conditioning and Renewables Interface

Subtask 3-1: Power electronics

The goal of this task is to look for innovative ways to reduce the cost of the cell stack power supply and associated electronics as well as improving its efficiency. Overall system efficiencies such as cells vs. current will be investigated in order to determine the optimum cost per kW they can provide. Design work will look to integrate many of the parts of the current power electronics design into the two systems to eliminate redundant framework and components. In an effort to improve efficiency multiple designs will be investigated to ensure that the selected power supply is taking full advantage of the numerous technical advances in the power electronic field.

Subtask 3-2: Alternate energy inputs

The goal of this task is to look at various types of renewables input and ensure that PROTON has designed an interface that will allow them to take power directly from the renewable source. This task will not involve any full scale testing with renewables but will design the interface and factor the design considerations into the power electronic task described in Task 3-1.

Task 4: System Cost Reductions

Subtask 4-1: Circuit board

The goal of this task is to evolve the controllers that are currently used on-board the electrolyzers into a circuit board design that will also serve to eliminate many of the electrical control monitoring that currently requires many discrete components and quite a bit of labor to wire. This will take the board developed during FY2000 and evaluate it in an actual system to refine and finalize the design of the board. This board will then be further developed into a board for their larger HOGEN 380 system.

Subtask 4-2: Component cost reductions

Pressure vessels in the HOGEN system, including the hydrogen-water separator, are machined from 316 stainless steel plate and pipe stock and welded to make the completed assembly. Valves, gauges and other small hydrogen and water components are plumbed together in a discrete manner with many fittings. The goal of this task is to effect significant cost reductions in the HOGEN fluid system by going to a powdered metal 316SS casting for the hydrogen-water separator. Use of manifold mounting of components on the hydrogen water phase separator or by using an alternate component manifold will eliminate fittings and permit use of less costly manifold mount valves and components.

Task 5: Manufacture Cost Reduced Design

Subtask 5-1: Manufacture a HOGEN 40

This task will implement the cost reduction advances made above into a fully functional cost reduced design. It will continue to be modified over the later parts of the program as other cost reduction efforts materialize. The unit will be run internally at Proton.

**Hydrogen Production Through Electrolysis
PROTON Energy System, Inc.**

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Catalyst Deposition and Optimization						
Complete catalyst ink development		◆				
Spreading and testing of membranes				★		
Cell Stack Support Component Mods						
Complete design of cast parts			◆			
Procure cast parts				◆		
Integrate cast parts into stack					◆	
					◆	
Flow Fields						
Characterize materials				◆		
Procure materials					◆	
Begin testing of materials						◆
Simplified Stack Compression Concepts						
Concept design				◆		
Fabrication					◆	
Evaluation						◆
Power Electronics						
Investigate H40 power supply options with supplier		◆				
Implement any found savings			◆			
Investigate H38D power supply options with supplier			◆			
Alternate Energy Inputs						
Investigate alternate energy inputs	◆					
Develop specification for input to HOGEN products			◆			
Circuit Board						
Complete H40 board specification	◆					
Complete H40 board design		◆				
Complete H40 board testing			★			
Complete H380 board specification				◆		
Complete H380 board design						◆
System Cost Reductions						
Complete system gas drying development				◆		
Complete casting design for H40			◆			
Complete manifolding design for H40			◆			
Complete casting and manifold prototypes					◆	
Manufacturer Cost Reduced Design						
Begin component procurement		◆				
Complete system assembly of H40		◆				

Task Designation/Milestone		2001				2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Integrate control board		◆				
Integrate gas drying				◆		
Integrate casting and manifolds					◆	
FY 2001 Begins October 1, 2000						

Renewable Hydrogen System Integration and Performance Modeling – Desert Research Institute

Desert Research Institute (DRI) has designed, purchased equipment, and built a system to use renewable energy (solar and wind) to produce electricity which is used to generate hydrogen for utilization in a fuel cell. The system was developed for use in remote areas with abundant but intermittent wind and/or solar energy so that renewable energy could be stored and used to produce electricity on demand. The system was built but the evaluation and modeling to optimize the operation was not completed.

The first task involved an evaluation of the system components and was completed in FY 2000. The remaining tasks include:

Task 2: Complete the System Assembly and Testing

The system is functional but still needs some additional work so that it will operate reliably and in a more automated manner. The system will be completed generally as initially designed with a few changes dictated by the lessons learned to date. The solar collectors, wind generators, inverter, battery system, electrolyzer, and hydrogen storage tank are all professionally installed and function properly. The fuel cell and the data acquisition and control computer need additional work. This task will complete the installation of the fuel cell and controller into the system. The data collection system designed will be completed, the installation finished, the entire system tested, and operators will be trained on the system. Performance and reliability data will be collected for at least six months. Up to three months of data is needed to provide for system optimization in Task 3. The system will be set up to capture all the data needed to manage the system and also to analyze the system performance.

Task 3: Develop the Models for System Control and Optimization

The system needs to be designed to function in an automated mode. This will be accomplished by developing computer software that will control and optimize the system function within the design parameters. The system performance will be evaluated with a load designed to simulate household use. The computer will be programmed, probably using TRNSYS as the platform, to control the system function. At least three months of performance data (of the six month total) will be collected with the operating and optimization software in place. A final report will be prepared describing the system and how it functions, data collection methodology system performance and reliability, and the logic control for the entire system.

Renewable Hydrogen System Integration and Performance Modeling Desert Research Institute						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Complete the System Assembly and Testing						
System made totally functional in a semi-automated state			◆			
Performance and reliability data collected			◆			
Develop the Models for System Control and Optimization						
Software development and testing completed			◆			
Data collected on system performance and reliability				◆		
Final report issued to DOE					◆	
FY 2001 Begins October 1, 2000		Critical milestone is to be determined				

Integrated PV- Electrolysis/ Metal Hydride Hydrogen Generation and Storage System for Scooter Applications - Energy Conversion Devices, Inc

Hydrogen is an ideal energy carrier, and can be produced through electrolysis from renewable energy resources, such as solar, wind, and biomass. Since renewable energy resources are wide spread and distributed in nature, renewable hydrogen may lead the way to commercializing a hydrogen infrastructure. The project is divided into three sections: production, storage, and utilization of renewable hydrogen. The objective of the project is to resolve integration issues for a renewable electricity generation /electrolyzer /metal hydride storage system; analyze the technical and commercial merit of such a system; and demonstrate a four-stroke scooter fueled by hydrogen. In addition to identifying cost competitive renewable hydrogen, the project also aims to establish strategic collaborations to manufacture and market these systems.

Phase I of the project resulted in a market study of the two wheeler (scooter) with particular emphasis on developing countries like India. During Phase II work Energy Conversion Devices (ECD) performed R&D of the component technologies and the integrated system, identified some integration problems, and also performed a preliminary economic analysis of renewable hydrogen from bagasse cogeneration. Phase III tasks are listed below and the critical milestones are indicated on the attached Gantt chart. Phase III commences on September 1, 2000.

Task 1: Optimization of Hydrogen Storage Materials

Subtask 1-1: Improve reversible hydrogen storage capacity

Up to 3.5 wt% absorption was found in some alloys prepared during phase II. Alloy R&D will focus on improvement of the desorption capacity.

Subtask 1-2: Study thermodynamic and kinetic properties

The reversible storage capacity, plateau pressure, enthalpy and entropy of reaction, and reaction rate constant will be determined using a Sievert's apparatus for alloys having high capacity.

Subtask 1-3: Improve moisture resistance

The main impurity of electrolytic hydrogen is moisture that can reduce the cycle life of the metal hydrides. Improved moisture resistance of the hydrogen storage alloy will result in simplification and cost reduction of the overall system.

Subtask 1-4: Scale up material production

Select alloys will be studied for reproducibility and scale-up that is critical for commercialization.

Task 2: Hydrogen Storage System Design and Performance Optimization

Subtask 2-1: Reduce system weight

The system weight reduction effort will be based on system design, and material selection. The design will be also include optimization for performance, safety and reliability

Subtask 2-2: Address heat and mass transfer

Means to enhance heat transfer with the surrounding medium and hydrogen transport within the storage system will be addressed.

Subtask 2-3: Evaluate metal hydride storage module

Metal hydride storage modules will be tested under different experimental parameters. Emphasis will be on characterizing the storage system for hydrogen ICE scooter application.

Task 3: PEM Electrolyzer – Metal Hydride IntegrationSubtask 3-1: Procure PEM electrolyzer

PEM electrolyzer will be procured from Proton Energy System.

Integrated PV-Electrolysis/Metal Hydride Hydrogen Generation and Storage System Ro Scooter Applications Energy Conversion Devices, Inc.						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Optimization of Hydrogen Storage Materials						
Improve reversible hydrogen storage capacity				◆		
Study thermodynamic and kinetic properties				◆		
Improve moisture resistance		◆				
Scale-up material production				◆		
Storage System Design and Performance Optimization						
Reduce system weight		◆				
Address heat and mass transfer		◆				
Evaluate metal hydride storage module			◆			
PEM Electrolyzer – Metal Hydride Integration						
Procure PEM electrolyzer	★					
Integrate electrolyzer with storage module		◆				
Analyze the techno-economics of a PEM electrolyzer – MH system			◆			
Metal Hydride – HICE Integration						
Convert a four stroke ICE from gasoline to hydrogen		★				
Conduct safety analysis			◆			
Business Plan/Economic Analysis of Bagasse Cogeneration – Electrolytic Hydrogen						
Identify business partners		★				

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Subtask 3-2: Integrate electrolyzer with storage module

The characteristics of the component technologies will be evaluated and technical specifications will be drawn out. The two technologies will be integrated and optimized for performance and cost. Performance parameters (hydrogen pressure, purity, flow rate, alloy PCT, storage system design) of the integrated system will be analyzed.

Subtask 3-3: Analyze the Techno-economics of PEM electrolyzer/metal hydride system

This sub-task will include analyzing the system specification, and the capital, operating and maintenance costs of the integrated system to arrive at a realistic economic evaluation.

Task 4: Metal Hydride H – ICE IntegrationSubtask 4-1: Convert a four stroke ICE from gasoline to hydrogen and evaluate performance

This subtask will convert a Honda Elite 80-cc scooter from gasoline to hydrogen. Dyno tests will be performed.

Subtask 4-2: Conduct Safety Analysis

Preliminary safety analysis will be performed on the HICE and metal hydride storage system with respect to hydrogen pressure management, corrosion, material suitability, and structural integrity to stress and vibration.

Task 5: Business Plan/Economic Analysis of Bagasse Cogeneration HydrogenSubtask 5-1: Identify business partners

ECD will seek collaboration for renewable hydrogen commercialization with an electrolyzer manufacturer, a sugar mill cogeneration plant in India, and a scooter manufacturer.

Hydrogen-Based Utility Energy Storage System – SRT Group, Inc.

The SRT Group will manufacturer and test a 50 kW Prototype Electrolysis System and demonstrated the unit to determine potential electrode lifetimes, achievable current density, and optimum operating parameters. Data from tests will be collected and analyzed for future system expansion.

Task 1: 50kW Prototype Electrolysis System

A preliminary design and system design will be developed for the major components required for the energy storage system. Specifications for the system will be determined and reviewed. The conceptual system designs produced by SRT will be reviewed and evaluated for consistency, safety, and the ability to manufacture parts from the drawings. After completion of the design work, the 50 kW electrolyzer unit will be manufactured.

Task 2: Test Stand, 50 kW Unit, Installation and Testing

In this task the Test Stand for the Electrolysis unit will be designed, fabricated, and delivered to the facilities in Latham, NY. A final report documenting this will be issued.

Task 3: Safety

A System Safety Analysis will be performed, this will include a design assessment, fabrication evaluation, evaluation of operating procedure, and a risk assessment. The system will require careful attention to process and equipment safety, with passive safety devices preferred over active ones.

Task 4: Facility Preparation

A facility will be prepared that will test the 50 kW Electrolyzer unit.

A Gantt chart and critical milestone are to be determined.

HYDROGEN INFRASTRUCTURE

Filling up with Hydrogen 2000 – Stuart Energy Systems

Under the program “Filling Up With Hydrogen 2000” hydrogen vehicle re-fueling systems, called fuel appliances will be developed in a prototype development program, which builds on Stuart’s new CST electrolysis technology. The fuel appliance combines the components needed to convert water and electricity to high-pressure hydrogen gas. The system consists of an electrolyzer, compressor and refueling dispenser packaged in one or more, easy to deploy units. The fuel appliance systems can be built to suit a wide range of hydrogen supply capacities, from the size needed to fuel a single vehicle over night, Personal Fuel Appliance (PFA), to larger service stations, Packaged Hydrogen Supply Appliances, which can support many vehicles, including large fleets of buses.

Task 1: Personal Fuel Appliance (PFA)

The second working model, P1 Model 25, producing up to 50 SCFH at 3600 psig, was built and successfully tested. Three versions of the P1 Model 25 have been built. The units have been taken to Detroit and Washington DC and demonstrated to North American automakers and the DOE. A purchase order has been received from Ford Motor Co. for the joint evaluation of personal fuel appliances over the next 30 month period. The first unit will be delivered to Ford in Q1 2001. The exchange of technical information on performance of these prototypes will complete this task.

Task 2: Packaged Hydrogen Fuel Appliances

Subtask 2-1: P3-1A Working Model

The working model P3-1A, featuring Stuart’s CST Multi-stack electrolyzer technology, is currently providing fuel for a fleet of hydrogen and Hythane vehicles including an Xcellsis P4 fuel cell bus. The unit will operate at SunLine Transit until March 31, 2003.

Subtask 2-2: P3-1B Working Model (2)

Unlike P3-1A, which uses Stuart’s CST Multi-stack Electrolyzer technology, P3-1B will use a train of CST Single-Stack electrolyzer. Two units of 400 SCFH were built in FY 2000. The first unit, P3-1A1, produces 400 SCFH at low pressure (200 psig) and has completed 2000 hours of factory testing. One of the two stacks on this unit has been disassembled and is undergoing evaluation. The unit will be reassembled and placed in the field. Discussions are on-going to deploy this unit at a site fueling hydrogen powered mining vehicles (Fuel Cell Propulsion Institute). These vehicles will use low pressure metal hydride gas storage.

The second unit, P3-1B2, capable of achieving 400 SCFH at 5000 psig is just started reliability testing, and will be deployed in hydrogen vehicle demonstrations expected to start in Q2 2001 in California.

Subtask 2-3: P3-5 Working Model

This task is scaled back from the original proposal. The scope of work has been reduced to design of the CST Multi-Stack electrolyzer cell stack to be used in these larger fuelers, and follows the change in plan approved by the DOE in August 2000. The construction of large fuelers has been deferred to the construction of the P4-10 Prototype Bus Fueller.

Task 3: Fueler Prototypes

Subtask 3-1: P4-1A Prototype(s)

Two P4-1 fuelers with a total capacity of 1000 SCFH will be built based on the P4 process technology and updated CST single stack electrolyzer. Similar to the process used in the personal fuel appliance the P4 prototypes will operate at higher cell pressures using a new pressure control system. The P4 process was successfully demonstrated on a large single stack electrolyzer. The design of the high pressure version of the system, which will produce hydrogen at a rate of 500, SCFH at 6000 psig is underway. Construction of the prototype is planned for Q2 2001. Field deployment of these units is to be decided later.

Subtask 3-2: P4-10 Prototype Bus Fueler

One large bus fueler capable of fueling up to 10 buses is scheduled to be built in Q4 2001/ Q1 2002. The unit will use the CST Multi-Stack electrolyzer and will produce up to 15,000 SCFH at 5000 psig.

Filling Up With Hydrogen 2000 Stuart Energy Systems						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Personal Fuel Appliance						
Deliver PI Model 25 to Ford Motor Company for joint evaluation		★				
Packaged Hydrogen Fuel Appliance						
Annual report on operation of P3 fueler at SunLine Transit				◆		
Deliver P3-1B1 to prototype test site				◆		
Deliver P3-1B2 to prototype test site				◆		
Complete cell stack design for P3-5 appliance		◆				
Fueler Prototypes						
Design and build P4-1 appliances				★		
Design P4-10 appliance						◆
FY 2001 Begins October 1, 2000						

Light, Medium Duty Fleet – NRG Technologies

NRG Technologies will work to bring clean, high-performance light to medium-duty vehicles using hydrogen fuels to market. Accomplishing this goal involves achieving many objectives. The first is to develop a cost-effective, low-emissions retrofit package for light to medium-duty vehicles that seamlessly converts existing natural gas and/or gasoline engines to hydrogen-enriched fuels. The second objective is exceeding California Air Resource Board Super Low Emission Vehicle (CARB SULEV) standards for 2003 using the Supplemental Federal Test Procedure (SFTP). Previous work by NRG Technologies has shown the following emissions levels. Carbon monoxide (CO) emissions will be undetectable (<1ppm); non-methane hydrocarbon (NMHC) emissions will be <0.05 g/hp-hr; and oxides of nitrogen (NO_x) will be <0.15 g/hp-hr. Depending upon the driving cycle, these values represent an 85% reduction in NO_x emissions alone when compared to the standard. NRG will also work to maintain or enhance current vehicle drivability, durability and operating range by effective selection, matching, and configuring of off-the-shelf components. They will also prove and enhance the retrofit package design through in-service testing. The final objective is developing a public/private partnership to implement a commercialization plan that will bring new business and economic opportunities to Nevada.

Task 7: Finalize Retrofit Package Design

Implementing the detailed test plan developed in Task 4, NRG will test the different packages developed in Task 3 to determine which designs deliver the best combination of engine power, low exhaust emissions, and fuel efficiency.

Task 8: Installation and Emissions Verification of Retrofit Packages

NRG will install the finalized engine retrofit packages on one Bechtel-supplied light duty vehicle and either the City of Las Vegas dump truck or the RTC paratransit bus. Once completed, each vehicle will be transported to CAVTC's facility in Hayward, CA. Each vehicle will be emissions certified to the 2003 SFTP driving test for that class of vehicle. Once this testing is completed. Both vehicles will be returned to Las Vegas for in-service testing.

Task 9: Federal, State and Local Approvals

NRG will conduct the required research to verify what, if any, approvals for operation of both the light and medium duty vehicles in their intended operation. It is anticipated that a temporary EPA exemption from the anti-tampering regulations will be obtained. Once the emissions levels of the retrofit packages are established, NRG will begin the process of obtaining EPA approval under Memo 1A.

Task 10: In Service Testing

Implementing the test plan developed in Task 4, NRG will manage the collection of data, both objective and subjective, for the operation of the two retrofitted vehicles.

Task 11: Vehicle Emissions Testing

Following in service testing of each retrofit package, the two vehicles will be returned to CAVTC. Here the driving tests will be repeated to determine the reliability of the emissions control technology.

**Light, Medium Duty Fleet
NRG Technologies**

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Finalize Retrofit Package Design	◆					
Installation and Emissions Verification of Retrofit Packages	◆					
Federal, State and Local Approvals	◆					
In Service Training				◆		
Vehicle Emission Testing				◆		
Verification of Vehicle Performance	★					

FY 2001 Begins October 1, 2000

Hydrogen Commercialization For the 21st Century - Sunline Services Group

This project is designed to transpose Department of Energy funded research & Development (alpha site) technology, in the area of hydrogen fuel development, to the next level in the process of full commercialization (beta site) infrastructure development. The project aims to generate hydrogen, from the renewable resources of solar and wind energy, to fuel a growing cluster of vehicles in the Coachella Valley Clean Cities Region.

During FY 1999/2000, SunLine Services Group completed system design, integration, and received permits to construct a commercial hydrogen generation facility. This was followed by construction of the hydrogen generation building, hydrogen vehicle garage, multi-purpose educational facility. The project incorporated two differing types of electrolyzers: (1) a Stuart Energy Systems electrolyzer that produces 1400 standard cubic feet (scf) of hydrogen per hour and (2) a Teledyne Brown electrolyzer that produces 40 scf of hydrogen per hour. Power is provided by renewable solar resources: (1) a flat plate array of solar panels from Siemens and (2) power from the Imperial Irrigation District. In preparation for the installation of photovoltaic tracking solar arrays they were manufactured and stored until the supporting structure could be completed. Storage and Dispensing Equipment was installed. There are two 4000psi tanks (12,000 scf) installed along with a mobile trailer with sixteen 3130 psi (104,000 scf) tanks. The dispensing unit contains two dispensers – one for hydrogen and one for a mixture of hydrogen and compressed natural gas known as Hythane[®].

Task 1: Integrate a Natural Gas Reformer into the Current System for Producing Hydrogen from Natural Gas

Task 2: Construct the Base Supports and Superstructure for the Photovoltaic Tracking Arrays

Install tracking arrays, integrate into the electrical system/grid and perform functional testing with installed equipment.

Task 3: Operations and Maintenance - Operate and Maintain a Fleet Of Hydrogen Powered Vehicles

Task 4: Documentation and Reporting

Develop a training curriculum to support the various equipment for production, storage, and dispensing of hydrogen as well as support the various power train configurations.

Hydrogen Commercialization for the 21 st Century Sunline Services Group						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Integrate natural gas reformer		◆				
Photovoltaic tracking arrays operational		★				
Operate and maintain equipment					◆	
Documentation and reporting				◆		
Training					◆	
FY 2001 Begins October 1, 2000						

Task 5: Training

Deliver training to sustain the cluster of hydrogen vehicles, as well as hydrogen production, storage, and dispensing equipment.

Hydrogen Reformer, Fuel Cell Power Plant and Vehicle Refueling System – Air Products and Chemicals, Inc.

Air Products and Chemicals, Inc., in partnership with Plug Power Inc. and the City of Las Vegas (CLV), Nevada, will develop a facility to serve as a commercial demonstration of hydrogen as a safe and clean energy alternative for vehicle refueling. The project objectives are:

- the development and demonstration of small-scale, on-site hydrogen production technology;
- design and installation of a hydrogen and hydrogen/compressed natural gas (CNG) blend refueling facility in Las Vegas, Nevada;
- the development and installation of a 50-kW PEM fuel cell system (FCS) at the Nevada site to be performed by Plug Power Inc.

Task 1: Design and Development

An existing hydrogen generator prototype will be tested to ensure its design, operation and system capabilities for integration with the FCS and the fuel station at the CLV site. A scaled-up hydrogen generator of sufficient capacity to meet the future demands at the CLV site will be designed based on the test results of the prototype. This generator will be sufficient to meet the hydrogen demand of the planned 27 vehicles, the 50 kW fuel cell system, and a 100 kW blended hydrogen/natural gas stationary engine/generator.

A 50 kW PEM FCS will be designed and developed. All aspects of integration of the FCS with the hydrogen production and compression system, and the integration of the FCS with site grid power will be worked out to arrive at a suitable FCS design.

A hydrogen and hydrogen/natural gas blend-fuel station will be designed to closely resemble the state-of-the-art in CNG fueling. The hydrogen generator(s) and 50 kW PEM FCS will be incorporated into this refueling station. A detailed design for the integration of the various subsystems will be completed to ensure that the components function smoothly as a total system.

Task 2: Construction and Installation

Initially, Air Products and CLV will install a fueling system to provide sufficient hydrogen to enable operation of three light-duty vehicles and the DOE H₂ hybrid electric bus. This system will consist of a merchant (liquid) hydrogen supply system, and the compression, blending, and fuel transfer equipment. In Phases 2 and 3, this fuel station will be integrated with the prototype, and subsequently the scaled-up hydrogen generators.

The prototype hydrogen generator will be moved from Allentown, Pa., reinstalled, and tied in to the FCPP, and fuel station at the Las Vegas site. As the demand for hydrogen grows sufficiently to warrant it, the scaled-up hydrogen generator will be assembled, installed, and integrated with the fuel station and the other loads at the site.

The 50 kW FCS will be assembled and tested at the Plug Power facility in Latham, N.Y., installed at the CLV site in Las Vegas, and connected with the hydrogen generator and fuel station subsystems.

Task 3: Systems/Station Integration

Permitting and safety review activities will be performed to install and operate the system at the site. Start-up and testing of the subcomponents to ensure proper operation will be completed. CLV, with assistance from Air Products and Plug Power, will operate and maintain the facility, ensuring that all subcomponents operate together as a whole and that the system has the highest level of availability and reliability. It is anticipated that from January 2002 onwards, as many as 27 vehicles will be refueling at the station.

The initial fueling system will be installed and on-stream. This system comprises a merchant liquid hydrogen supply system, and the compression, blending, and fuel transfer equipment.

After completion of a testing program in support of the development and design of the scaled-up hydrogen generator, the prototype hydrogen generator will be moved from Allentown, Pa. to Las Vegas, installed and integrated with the fuel station.

The 50 kW FCS will be designed, assembled, tested and then shipped to Las Vegas to be connected with the hydrogen generator and fuel station. Air Products, CLV, and Plug Power will conduct the start-up testing of the various subcomponents after installation at the site. They will ensure that all subcomponents operate together as a whole and that the system has the highest level of availability and reliability.

Hydrogen Reformer, Fuel Cell Generator, and Vehicle Refueling System Air Products and Chemicals, Inc.

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Reformer Design Development						
Complete prototype generator testing		◆				
Complete design of scaled-up commercial hydrogen generator			◆			
Decision point to fabricate and assemble a scaled-up hydrogen generator					◆	
50 kW PEM Fuel Cell						
Complete design of 50 kW PEM fuel cell system		◆				
Assembly complete			◆			
Performance test complete at Plug Power			◆			
CLV Vehicle Refueling Station						
Design of vehicle refueling station completed	◆					
Deliver equipment to site		◆				
Construction and Installation						
Commission refueling station in Las Vegas (based on liquid hydrogen supply source)		◆				
Commission hydrogen generator at CLV refueling station				★		
Commission 50 kW PEM fuel cell at CLV refueling station				★		

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Reliability data from the various subcomponents will be gathered, and the need for any corrective actions will be determined. Valuable experience will be gained on the usage patterns of the fuel station, and on the ease of use of the fuel-dispensing systems, which will indicate if any modifications need to be made in the later phases of operation.

A decision will be made on the feasibility and need for construction of the scaled-up hydrogen generator.

Hydrogen Composite Tank Program - IMPCO

The purpose of this project is to design, develop, prototype, and produce lightweight production hydrogen tanks and regulator valves that will be retrofitted for demonstration on two vehicle programs. The hydrogen tanks will be used on a public transportation bus and on two sport utility (SUV) vehicles

Phases I through IV have been complete prior to FY 2001.

Task 1: Phase V

Materials, tools, and the technical expertise to develop, design, test, certify and fabricate the hydrogen tanks and regulators will be provided. The original designs, design changes, manufacturing methods, improvements in manufacturing and any test results obtained will be provided to the U.S. Department of Energy (DOE). In addition, the manufacturing process histories and process parameters for all test articles will be provided to DOE.

Subtask 1-2: In-Tank Regulators

This task will validate the current design IMPCO in-tank regulator to NGV3.1 and PRD-1 standards for hydrogen. The in-tank regulators and 25 tanks will be supplied to DOE. Leak checking and field replacement of these regulators shall be performable by demonstration project personnel, who will be trained by the contractor in the minimal list of operations required to verify and replace faulty regulators.

Subtask 1-2: Reports

The contractor will provide monthly reports and a final report describing the design and testing of IMPCO regulators any design changes necessary to meet NGV3.1 and PRD-1 to DOE.

Task 2: Phase VI

Process development will be performed to increase pressure rating of tanks and improve the percent hydrogen by weight to produce 14 prototype hydrogen tanks. Process development can take place at the smaller length. Two separate batches, 10 prototype hydrogen tanks, will be fabricated and tested at the shorter length. The knowledge gained in the testing of the first fabrication batch will be used to feed back into the design for the second batch. The remaining four hydrogen tanks will be fabricated and tested in accordance with the specifications at the longer length. All prototype hydrogen tanks in this phase shall be tested to destruction. The knowledge gained from this task will be used to develop two frozen designs that of meet the NGV2 requirements, including the modified HGV2 requirements, dimensional specifications, and percent hydrogen by weight specifications.

Subtask 2-1: Reports

Monthly reports as well as a final report will be provided to DOE describing the testing of the 14 hydrogen tanks in this task and the frozen hydrogen tank design to be used for Task 3.

Task 3: Phase VII

Twenty identical hydrogen tanks of the 11 inch OD x 69 inch length and eight identical hydrogen tanks of the 11 inch OD x 93 inch length will be produced. The first 14 of 20 hydrogen tanks produced at the 69-inch length and the first 2 hydrogen tanks of the 93 inch length will be used for NGV2 certification. Four hydrogen tanks of each length will be delivered to a demonstration program to be determined by DOE

and the additional set of two hydrogen tanks of each length will be delivered to Lawrence Livermore National Laboratory, Livermore, CA, by first quarter FY 2002.

Subtask 3-1: Reports

Monthly reports as well as a final report will be provided to DOE describing the tank fabrication progress and the NGV2 certification test results.

Hydrogen Tank Program IMPCO						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Phase V						
Validate 5 ksi manual valve to NGV 3.1	◆					
Validate 5 ksi manual valve to PRD-1	◆					
Validate in-tank regulator to NGV 3.1		◆				
Validate in-tank regulator to PRD-1		◆				
Deliver 12 manual valves		◆				
Deliver 17 in-tank regulators			◆			
Phase VI						
Liner development		◆				
Seal development		◆				
Composite shell development			◆			
Full scale tank development and testing			◆			
Prepare reports			◆			
Phase VII						
Fabricate tanks				◆		
Perform NGV2 testing					◆	
Ship tanks					◆	
Final Report						◆
Phase VIII						
Design and development						
Validate in-tank regulator to NGV 3.1				◆		
Validate in tank regulator to PRD-1					◆	
Deliver 12 in-tank regulators						◆
Final report						◆

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Critical milestone is to be determined

Task 4: Phase VIII

The current design IMPCO in-tank regulator will be modified to NGV3.1 and PRD-1 standards for hydrogen. A total of 16 regulators, four will be for testing and spares, shall be supplied to DOE along with each of the 12 tanks delivered in Phase VII. Leak checking and field replacement of these regulators will be performable by demonstration project personnel, who will be trained in the minimal list of operations required to verify and replace faulty regulators.

Subtask 4-1: Reports

Monthly reports as well as a final report will be provided to DOE describing the design and testing of IMPCO regulators in this task and any design changes necessary to meet NGV3.1 and PRD-1.

Insulated Pressure Vessels for Vehicular Hydrogen Storage – Lawrence Livermore National Laboratory

The purpose of this project is to design, analyze, construct and test low-temperature, high-pressure gaseous hydrogen storage vessels. These vessels should be capable of handling temperatures as low as 20 K and pressures as high as 34.4 MPa (5000 psi). These vessels have packaging characteristics similar to those of conventional, low-pressure liquid hydrogen tanks, with much reduced venting losses. Compared with liquid hydrogen, cryogenic high-pressure hydrogen gas gives increased flexibility to the fueling infrastructure, since the vehicle can be fueled with liquid hydrogen, with high-pressure hydrogen cooled with liquid nitrogen, or with hydrogen at ambient temperature. Other forms of hydrogen storage exist, but they have their limitations. Hydride storage is heavy, and compressed hydrogen requires a very large volume.

This project aims to develop and demonstrate a near-term storage technology that can satisfy light duty vehicle storage needs in a cost effective way. The insulated pressure vessel can be used in light duty vehicles, storing 5 kg of hydrogen and resulting in a long range (640 km), low weight (30 kg), and low external volume (140 liters), and no hydrogen losses due to venting under all but the most extreme conditions.

Other advantages of insulated pressure vessels are:

- They can reduce the total requirement for liquid hydrogen, because they have the potential to use ambient-temperature-compressed hydrogen under most conditions. Liquid hydrogen may only be used when a long range is required.
- Insulation requirements are significantly reduced from those of a liquid hydrogen tank. This reduces the cost and the thickness of the insulation. As a result, the external volume of a cryogenic pressure vessel is likely to be lower than the external volume of a conventional liquid hydrogen tank.

Task 1: Deliver Pressure Vessels

LLNL will deliver 4 insulated pressure vessels to Structural Composites Industries (SCI) for testing. The vessels will be tested according to the DOT standards. The tests conducted will consist of: cycling, ambient temperature; cycling, environmental; cycling, thermal, and gunfire.

Task 2: Validate Finite Element Model

LLNL will validate the results of the finite element model by using the experimental results for temperature, pressure, and strain. Results from the finite element model should indicate that no damage to the vessel results from low temperature operation.

Task 3: Identify a Vehicle Demonstration Project

LLNL will work in finding a vehicular demonstration project that is relevant to the Hydrogen Program where the insulated pressure vessel can be installed and used.

Task 4: Propose a Procedure for Obtaining Insulated Pressure Vessel Certification

A draft procedure will be generated for certifying insulated pressure vessels. This draft procedure will then be distributed to industry for comment and later submitted to regulatory bodies (DOT, SAE) for their consideration.

Task 5: Build Full Size Vessels

LLNL will build 6 full-size (130-liter internal volume) insulated pressure vessels according to thier current design.

Task 6: Test Vessels to DOT/SAE Standards

LLNL will test their full-size vessels according to the DOT and SAE standards. They will conduct the following tests: if the budget is \$450K, drop from three and ten meters; if the budget is \$500K, they will also do the two bonfire tests (SAE bonfire test and DOT bonfire test).

Insulated Pressure Vessel for Vehicular Hydrogen Storage Lawrence Livermore National Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Deliver Pressure Vessels						
Four insulated pressure vessels will be delivered for testing according to DOT standards	◆					
Validate Finite Element Model						
Finite element model will be validated using experimental results			◆			
Identify a Vehicle Demonstration Project						
Identify a project appropriate for tank installation and use				◆		
Propose a Procedure for Obtaining Insulated Pressure Vessel Certification						
Draft procedure will be distributed to industry and regulatory agencies for comment				◆		
Build Full Size Vessels						
Six full size 130 liter insulated pressure vessels will be built					★	
Test Vessels to DOT/SAE Standards						
Full size vessels will be tested by drop and bonfire tests						◆

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OTT Solicitations – TBD

The U.S. Department of Energy's Office of Transportation Technologies (OTT) together with the Hydrogen Program is developing both on-board chemical storage systems for hydrogen and off-board reforming and refueling systems. Reformate from a typical autothermal or partial oxidation (POX) fuel processor operating on methanol, ethanol, natural gas, or a petroleum-based fuel is composed of approximately 40% hydrogen (dry basis). The balance is primarily CO₂ and nitrogen, which act as diluents in the hydrogen feed stream. A reformate must be processed to reduce CO content, which acts as a poison to PEM fuel cell catalyst, to approximately 10ppm under steady-state operating conditions. Other trace impurities that may be present at part-per-million levels in the reformate feed, such as hydrogen sulfide and ammonia, may also degrade fuel cell performance. OTT is developing innovative technologies and/or system configurations to concentrate the hydrogen content in a partially or fully reformed feed stream.

The long-term goal for fueling fuel cell-powered vehicles is to use hydrogen stored onboard the vehicle that is produced from renewable feedstocks and dispensed at refueling stations. An interim path to this vision is to reform natural gas or gasoline products at refueling sites to generate hydrogen, which would then be stored and dispensed. Such distributed refueling stations would need to provide hydrogen at a cost that is competitive with gasoline used for cars powered by internal combustion engines. OTT is involved in developing a cost-effective method of off-board hydrogen reforming technologies.

Task 1: On-Board/Off-Board Hydrogen Enhancement

The purpose of this task is to enhance the hydrogen content in on-board and off-board fuel cell feed streams. This involves a technical concept and system analysis and feasibility assessment addressing system efficiency, possible pressure differential issues, and complexity. An economic/cost analysis and a benefits and risk assessment will also be conducted. A proof-of-concept demonstration will be done followed by fabrication and testing of prototype hardware that will be validated in a fuel cell power system.

Task 2: Advanced Chemical Hydride On-Board Storage Systems

In this task, an on-board hydrogen supply/storage system will be developed. It will be capable of being installed and operated in a PNGV-class sedan (or other similar vehicles included in other DOE demonstration programs). It will meet a series of technical targets including six percent of system hydrogen weight, an energy density of 1500 watt hours per liter, and a specific energy of 2000 watt hours per kilogram. It will be viable for 500 refueling cycles and will cost \$1 per kWh under mass production.

Task 3: Advanced Chemical Hydride Standardized Testing Procedures/Facilities

The objective of this task is to develop an independent testing capability and standardized test procedures for advanced chemical hydride storage system. Periodic reports on the performance of advanced materials will be delivered to an industry/government advising committee.

Task 4: Off-Board Hydrogen Reforming and Storage

The goal of this task is to design, develop, and demonstrate a small-scale reformer and refueling system that can produce hydrogen at a cost that is within five percent of the cost of premium gasoline and will have the potential of being mass produced. This reforming-refueling system will be sized to produce no

less than 40 to 60 kg of hydrogen per day at a delivered cost of approximately \$2.00 to \$ 2.50 per kg (pre-tax).

Subtask 4-1: Literature search, functional analysis, and conceptual design

This subtask includes a literature search, functional analysis, and a conceptual design for each of the major subsystems: reformer, hydrogen purification, compressor, storage and dispenser.

Subtask 4-2: Bench-scale research and development of high priority, selected subsystems, equipment and techniques

This subtask will involve bench-scale research and development of high priority, selected subsystems, equipment and techniques based on the performance targets established in subtask 4-1. The development areas include; low-cost reformers, improved cost-effective hydrogen purification technology, hydrogen storage technology, and high efficiency, low cost ancillary equipment for on-site reforming systems.

Subtask 4-3: Fabrication and testing of a full-scale integrated hydrogen production, storage, and dispensing system

A prototype system will be developed and sited at a vehicle fueling facility for third-part validation.

A Gantt chart and critical milestone are to be determined.

Refueling Infrastructure for Fuel Cell Underground Vehicles Including a Locomotive – TBD

The next technology step beyond the electric mine is the hydrogen mine. Hydrogen produced onsite is distributed underground and serves as the energy source for fuel cell vehicles and other machines. The Fuelcell Propulsion Institute, an international technical and educational consortium of 23 members structured as a nonprofit corporation, will develop and test the technology to make the hydrogen mine a reality.

The introduction of fuel cell mine vehicles requires that a hydrogen infrastructure will overlay the existing one. The system will provide onsite hydrogen production, distribution, and transfer to the hydride beds of the working vehicles, preferably at the point of operation. Fuel cells may also provide power for non-vehicular mining machines.

Underground locomotives are a unique crosscutting vehicle technology. Their applications can include metal mining, coal mining, tunneling, and construction. Fuelcell Propulsion Institute, with the assistance of H Power Corporation and Sandia National Laboratories/CA, is developing and testing the world's first fuel cell-powered underground vehicle, a mine locomotive.

Task 1: Refueling Infrastructure for Fuel Cell Underground Vehicles

The project will develop and evaluate technology for hydrogen production, distribution, and vehicle refueling in underground metal mines and tunneling.

Subtask 1-1: Feasibility analysis

In this subtask analytic methods will be used to determine the most practical and broadly applicable methods of hydrogen production for hardrock mining and tunneling, distribution within mines, and tunnels and vehicle refueling.

Subtask 1-2: Engineering design

Undertake engineering design of the highest-ranked method for each of the three subsystems (production, distribution, and refueling) for implementation in hardware and experimental evaluation.

Subtask 1-3: Production evaluation

Construct the hardware and experimentally evaluate the method(s) of hydrogen production established in subtask 1-1.

Subtask 1-4: Distribution evaluation

Construct the hardware and experimentally evaluate the method(s) of hydrogen distribution established in subtask 1-1.

Subtask 1-5: Refueling evaluation

Construct the hardware and experimentally evaluate the method(s) of vehicle refueling established in subtask 1-1.

Subtask 1-6: System design

Based on economic and safety analyses of specific mine test sites determine the most optimal hydrogen infrastructures based on the best subsystems evaluated in subtasks 1-3 – 1-5.

Subtask 1-7: Premining system validation

Safety of underground workers and non-disruption of mine operations require that systems be debugged prior to introduction into an operating mine. Each system designed in subtask 1-6 will be constructed and thoroughly evaluated for safety.

Subtask 1-8: Mining system validation

Validate one or more of the systems of subtask 1-7 in commercial mining operations.

Task 2: Locomotive ProjectSubtask 2-1: Design and fabrication

Fuelcell Propulsion Institute has developed a four-ton, 14kW hydride fuel cell locomotive derived from a battery vehicle of similar power. The fuel cell is a standard design of H Power Corporation; Sandia National Laboratories provided the hydride system. While matching or exceeding the battery in power, voltage, and current (tractive effort), the hydride fuel cell powerplant will be substantially lighter and have at least five times the volumetric energy density.

Subtask 2-2: Vehicle display

Following the completion of subtask 2-1, this vehicle will be displayed at the MINExpo INTERNATIONAL 2000, October 9 – 12, in Las Vegas, NV.

Subtask 2-3: Evaluation

Fuelcell Propulsion will execute safety, performance, and user-acceptance tests aboveground. They will also evaluate two potential refueling procedures using a hydride cylinder. Under the auspices of Canada Centre for Mineral and Energy Technology (CANMET), this subtask will evaluate the locomotive for productivity in mine operations underground.

Subtask 2-4: Final report

A final report will be issued to DOE upon the completion of this project.

A Gantt chart and critical milestone are to be determined.

REMOTE POWER

Alaska PEM Fuel Cell Validation Project – University of Alaska, Fairbanks

Work on the PEM fuel cell program currently funded under the Rural Alaskan Power Program, initiated in late FY 98 will continue in FY2001. The UAF Energy Center is designated as the test site for technologies supplied by other vendors. This work is in cooperation with Sandia National Laboratories at Livermore (SNLL), and multiple industrial partners.

This program had an extremely aggressive schedule during FY 2000, but has slipped from the timetable proposed a year ago. The major problem has been the lack of delivery of a reliable diesel reformer from any of three industrial suppliers. Given the lack of a reformer, the testing of integrated systems cannot be done. However, this program continues to make significant progress in assisting industrial partners with development of reformers and integrated fuel cell systems, as well as providing a fundamental understanding of the performance of these systems. This information is useful for determining the suitability of PEM stationary power systems for use in remote and distributed power applications.

To date, the program has been evaluating the performance of a PEM system based on a steam reformer integrated with a palladium membrane providing high purity hydrogen to a pure hydrogen PEM fuel cell. This system has the advantage of allowing the hydrogen to be used efficiently by the fuel cell stack. This system works well for short demonstrations in the laboratory, but does have several problems that must be solved before the system is sufficiently robust for a field trial.

It should be noted that the slower than expected progress in this program is entirely in line with recent statements coming from the PEM fuel cell industry. GE has announced that Plug Power has not met the specifications of the contract, and they are under no obligation to purchase units from them. IFC (the only company currently selling commercial fuel cell systems of any type) has entered the PEM field, but expects it to be four to six years before they have a commercial product ready for market.

This program is providing valuable information to the energy community by providing independent third party evaluations of the technology as it exists at this point in time. UAF hopes to continue to serve this function as the technology continues to evolve and grow.

Task 1: Evaluate Energy Balance on Autothermal Diesel Reformer supplied by Dais Analytical

Task 2: Evaluate Energy Balance of Fully Integrated PEM Fuel Cell System Supplied by Dais Analytical and Establish Integrity of Unit in Laboratory

Task 3: Develop Remote Monitoring Capability while Unit in Laboratory

Task 4: Begin Field Testing of Integrated Units

Task 5: Publish Results from Autothermal Reformer Evaluation

Task 6: Continue to Collect Energy Use Data from Alaskan Residences

Task 7: Evaluate Other Reforming Technologies in Conjunction with Sandia Livermore (RF Reformer)

Alaska PEM Fuel Cell Validation Project
University of Alaska, Fairbanks

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Evaluate autothermal reformer		◆				
Evaluate integrated diesel PEM system (in laboratory)			◆			
Determine suitability of system for field test			★			
Begin field test			◆			
Develop monitoring system			◆			
Publish results			◆		◆	

FY 2001 Begins October 1, 2000

Power Parks System Simulation Project – Sandia National Laboratories

Sandia National Laboratories will develop a system model to simulate distributed power generation in power parks, where power generation is co-located with a business or an industrial energy consumer. Due to deregulation, aging infrastructure, and increasing demand, the idea of distributed power generation in power parks is gaining interest nationwide. Power parks can be sited as a node on the electric grid in areas where local energy use or geographical factors make an alternative energy source practical. Proposed power parks might use combinations of technologies, such as photovoltaic collectors, wind turbines, gas micro-turbines, and fuel cells fed by hydrogen generated by electrolysis or hydrocarbon fueled reformers. Power parks provide an excellent opportunity for hydrogen technologies to contribute to the generation of electrical power.

The deliverable of the project will be a tool for simulation of the power generation system, constructed in the language of the Simulink software. We will develop a library of individual components for hydrogen production, storage, and utilization to generate electricity, along with components representing internal loads and electric distribution to the grid. These modules can then be extracted from the library to construct a system model for a specific power park. The Simulink software allows the components to be coupled in block diagram format, convenient for varying the configuration of the park. Dynamic simulations will predict the performance of the power park subject to variations in system parameters. Variations in the system design can be evaluated to optimize the power production and minimize energy consumption. Previous work at Sandia performed simulations for remote-area power systems consisting of a fuel-reformer, a fuel cell, and a hydrogen storage system to meet a load cycle. We also examined hydrogen and electrical storage (batteries) to match a periodic energy resource (solar energy) with a demand profile.

The project tasks will begin with development of the library of Simulink modules for the various components being proposed for power parks. Then the components will be assembled into a sample power park to evaluate performance of the system for power generation and energy efficiency. The sample power park will be based on existing or proposed parks, but not dedicated to a specific park. The energy use within the park will be based on a sample industrial process with sufficient generality in the definition of a load function that the results and experience gained will be useful for understanding other cases. Lastly, a control system will be implemented to direct the power to internal loads, to storage components, or to be distributed to the power grid. Previous experience with energy analysis of residential systems (S.R. Vosen, J.O. Keller, *Int. J. Hydrogen Energy*, 1999; 24: 1139-1156) showed that the control strategy affects the optimal design of the components, especially those related to energy storage; intelligent control allowed division of energy between storage options that yielded a system with lower-cost and higher efficiency.

Power Parks System Simulation Project Sandia National Laboratories						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Develop library of Simulink modules for power park components			◆			
Configure the component modules for a sample power park				◆		
Evaluate system performance on power and energy efficiency				◆		
Implement a control algorithm to optimize power park					◆	
FY 2001 Begins October 1, 2000						
Critical milestone is to be determined						

Alaskan PEM Fuel Cell Validation Projects – Sandia National Laboratories

Sandia National Laboratories is providing technical program management in support of a development and deployment remote area power program for Alaskan applications. Fuel utilization in remote Alaskan villages is far from optimal. Electrical power is generally produced from diesel generator sets resulting in a multitude of problems for example: this power is very expensive, unreliable, and results in air, ground and water pollution. The waste heat from these generator sets is often used to heat a large nearby building like a school, however, the individual dwelling owner does not directly benefit from this waste heat which frequently represents 60% of the overall energy requirements. This Alaskan Proton Exchange Membrane Fuel Cell (PEMFC) Program provides an opportunity to adapt developing PEMFC technologies to provide an integrated solution for improved fuel utilization for the arctic Alaskan villages.

One of the goals of this program is to provide PEMFC systems producing 3-5 kW of grid quality power engineered for remote applications in the arctic climate of Alaska. These PEMFC systems will be engineered to maximize fuel utilization addressing the dwellings entire energy needs, including all electrical, space and water heating needs. This will significantly reduce the overall energy consumption in Alaskan remote villages and increase electrical system reliability. As a transition strategy these first PEMFC systems are to be operated on hydrogen from reformulated diesel fuel. This will position the Alaskan villages to eventually replace the dependence on diesel fuel and shift to some other form of energy, for example, renewables.

There were three distinctly separate projects associated with phase I of this program. In phase II there was two projects. Each project is performed by a team of industrial partners in collaboration with Sandia National Laboratories, The Alaskan State Energy Office, and The University of Alaska at Fairbanks (UAF). This program is designed for a three phases execution. The first two phases have been completed, the third is stated below.

Phase 3:

A diesel reformer / PEMFC / Power conditioning system shall have the capability to provide power for a single structure (i.e. private residence or small commercial building). The Reformer / PEMFC / Power conditioning system will be part of a hybrid system using an energy storage system to supply the peaking needs of the application of choice. The size for this system will produce 3 - 5 kW base load. This system must be at least a pre-commercial prototype. The energy storage system will be designed to handle the peaking demand as determined by the end use. This system must be delivered, installed and made operational in the TBD Alaskan remote application between September 30, 2000 and December 31, 2000.

The performance of the reformation technologies fell short from what was first anticipated. As a result phase III has been stalled while SNL and UAF perform test and evaluation of the broadest spectrum of reformers obtainable. The reformers that are currently being investigated are steam reformation, autothermal reformation, and plasma reformation. The test and evaluation are focusing on determination of the controlling physics as opposed to engineering issues. If it is found that the performance of these devices can be improved through improved engineering to an acceptable level we will re-instate phase III. A first law analysis of these technologies is used as the limiting metric however; a detailed speciation of the effluent stream will also be performed subject to time and funding availability.

**Alaskan PEM Fuel Cell Validation Program
Sandia National Laboratories**

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Pre-prototype optimized fully automated PEMFC system delivered to UAF			◆			
Pre-prototype qualified by UAF for Alaska remote applications				◆		
Field testing to begin				◆		

FY 2001 Begins October 1, 2000

Critical milestone is to be determined

3.3 Analysis and Technology Transfer

This element includes projects in the areas of analysis (process, systems, and integration) and in the transfer of technology both domestically and internationally. Projects are being undertaken at universities, national laboratories, and in industry.

The analysis area is made up of projects involving analysis of technology development and validation processes, analysis of integrated systems, and integrated analysis of major components of the overall program. The systems analysis area consist of environmental, economic, and market analyses of potential hydrogen energy systems, their subcomponents, and the supporting infrastructure, as shown in Table 3.6. The products of these analytical studies will be used by the DOE Program Manager to establish program priorities for R&D as well as for near-, mid-, and long-term component, subsystem, and system validations.

Table 3.6 Analysis Projects		
Goals:		
<ul style="list-style-type: none"> • Ensure that Federal R&D investments in hydrogen production, storage, distribution, and end-use technologies will provide the maximum value added to national strategic goals including global greenhouse emission mitigation; • Identify and evaluate key market segments and market entry conditions for hydrogen utilization in transportation and in electricity generation at distributed and remote locations; and • Develop and apply metrics to measure the Program's contribution to attaining national strategic energy goals and market share in key market segments. 		
Category	Project	Research
<i>Analysis Activities</i>	Process Analysis of Hydrogen Research Activities	National Renewable Energy Laboratory
	Fuel Leak Simulation	University of Miami
	Distributed Hydrogen Fueling Systems Analysis	Directed Technologies, Inc.
	Strategic Response to Scenario Planning	National Renewable Energy Laboratory
	Hydrogen Technical Analysis	Arthur D. Little Inc.
	Billings Fuel Cell Project	Big Sky Economic Development
	Technoeconomic Analysis of Area 2 Hydrogen Production	Florida Solar Energy Center

ANALYSIS ACTIVITIES

Process Analysis of Hydrogen Research Activities – National Renewable Energy Laboratory

Process analysis provides direction, focus, and support to the development and introduction of hydrogen through evaluation of the technical, economic, and environmental aspects of hydrogen production technologies. Such analyses allow NREL to determine the prospects that a process will be economically competitive with conventional systems, and to identify opportunities that will result in cost reductions. Additionally, the environmental benefits of renewable technologies can be quantified and integrated with the economics of the process.

The technical, economic, and environmental aspects of technologies being researched in the Hydrogen Program are evaluated. Broadly speaking, two analysis methods are used to effect this work. First, technoeconomic analyses (TEA) are performed to determine the potential economic viability of a research process. Second, life cycle analysis (LCA) is used to evaluate the environmental benefits and drawbacks of the process.

Different levels of technoeconomic analyses are performed depending on the extent to which the system has been defined and the amount of data that has been generated. Results can include the minimum yields, maximum manufacturing costs, or necessary market conditions for the technology to be economically competitive, or may give the cost of the final product over the expected life of an industrial-scale plant.

The advantages of performing TEAs within a research environment are several fold. First, the economic feasibility of a project can be assessed by evaluating the costs of a given process compared to the current technology. These analyses can therefore be useful in determining which projects have the highest potential for near-, mid-, and long-term success. Second, the results of a TEA are useful in directing research toward areas in which improvements will result in the largest cost reductions. Finally, as the economics of a process are evaluated throughout the life of the project, advancement toward the final goal of commercialization can be measured.

The second analysis tool, LCA, is an analytic method for identifying, evaluating, and minimizing the environmental impacts of emissions and resource depletion associated with a specific process. When such an assessment is performed in conjunction with a technoeconomic feasibility study, the total economic and environmental benefits and drawbacks of a process can be quantified. Material and energy balances are used to quantify the emissions, resource depletion, and energy consumption of all processes required to make the process of interest operate, including raw material extraction, processing, and final disposal of products and by-products. The results of this inventory are then used to evaluate the environmental impacts of the process so that efforts can be focused on mitigating these effects.

Task 1: Analysis of New Projects, Funded or Proposed

As new projects are proposed for funding by the Hydrogen Program, they will be analyzed to determine their potential for economic viability. These analyses will likely be limited to cost boundary, and will include many alternative cases to take into account possible research advances. Work on this activity will be performed at the request of Hydrogen program management, as new project ideas are proposed.

Task 2: Assessment of Biological Hydrogen Production

A series of analyses will be performed to identify areas for potential improvement in biological hydrogen production systems. Systems to be studied include those being funded by the Hydrogen Program.

Task 3: Assessment of Thermocatalytic CO₂-Free Production of Hydrogen from Hydrocarbon Fuels

The process being developed at the Florida Solar Energy Center to thermocatalytically decompose hydrocarbon fuels in the absence of air and/or water to produce hydrogen and a carbon byproduct will be evaluated. Previous assessments conducted by the principal investigator will be reviewed, and new research data will be taken into account in a new analysis. A detailed process design of the system will be performed in order to provide information necessary to determine capital and operating costs. A cash flow analysis will determine the final cost of hydrogen, and a Monte Carlo sensitivity analysis will be used to identify the most critical variables.

Task 4: Assessment of the Mass Production of Carbon Nanotubes

Methods for mass-producing carbon nanotubes will be identified. Where available, costs will be applied to determine the cost of storing hydrogen, as a function of the expected storage capacity. A sensitivity analysis will be conducted to determine the range of storage prices given expected capacities.

Task 5: Assessment of the Cost of Mass-Produced Small-Scale Reformers

A review of past studies and literature available on the cost to mass-produce small-scale reformers will be carried out. The fuel to be reformed is assumed to be natural gas, for the purpose of near-term adoption of hydrogen in the transportation sector. Following a summary of the literature, a fresh analysis on the likely cost of such systems, including the effects of process efficiency, capacity factors, and required utilities integration, will be conducted.

Process Analysis of Hydrogen Research Activities National Renewable Energy Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Analysis of New Projects, Funded or Proposed						
Letter reports as needed					◆	
Assessment of Biological Hydrogen Production						
Report on analysis					★	
Assessment of Thermocatalytic Production of Hydrogen						
Report on analysis			◆			
Assessment of Mass-Production of Nanotubes						
Report on analysis				◆		
FY 2001 Begins October 1, 2000						

Fuel Leak Simulation – University of Miami

This project builds on a previous accident severity analysis utilizing a 1985 Mercury Cougar converted to compressed hydrogen storage. That work appears in the DOE video “Hydrogen: A Matter of Safety”. This work will produce a comparison of hydrogen fuel leakage to gasoline fuel leakage. Additionally, spectral analysis of the flame will be conducted.

Task 1: Production of Fuel Leakage and Ignition Video

The principal focus of this work is to show, through a high-quality video, the difference between a hydrogen fueled vehicle fire and a gasoline fueled vehicle fire. This will be accomplished by acquiring a recent, but damaged, production vehicle probably through auction. The vehicle will be modified by installing a hydrogen fuel compartment. The hydrogen fuel compartment will have an upper vent and be located between rear seat and the trunk. Hydrogen will be leaked from the fuel compartment, ignited, and videotaped. The vehicle will then be converted back to its gasoline-fueled configuration. Gasoline will be leaked from the fuel compartment, ignited, and videotaped. This will destroy the vehicle.

Task 2: Spectral Analysis of Hydrogen-Air Flame

Previous experiments with unrestricted hydrogen releases from vehicles have shown the flames to be easily seen on videotape if the experiments occur in the absence of sunlight. Researchers at Sandia National Labs and elsewhere have asked why hydrogen air flames are so easily seen on videotape. The intent of this task is to answer that question. Thoroughly pre-mixed hydrogen oxygen flames theoretically would not emit appreciable light in the visible range. The ignition of leaking hydrogen produces hydrogen air flames that have minimal pre-mixing. By measuring the wavelength of the light emitted by the flame it is probable the chemical reaction producing the light can be identified. This would allow the determination of whether flame visibility is due to impurities in the air (the hydrogen is ultra high purity) or inherent in all hydrogen air flames.

The eight steps to completion of the project are as follows:

1. Choosing an appropriate late model vehicle for conversion to hydrogen operation.
2. Locate and purchase the vehicle. Estimated cost of the vehicle is \$4000. The vehicle will probably be bought at auction.
3. Locate and prepare facility for leak accident simulations. The facility used for two previous vehicles will probably be used again.
4. Install the hydrogen fuel compartment in subject vehicle. This is a process that has been done previously. The modification includes changes to the stock trunk lid.
5. Perform a hydrogen leak accident simulation. This involves the simulated puncture of a compressed hydrogen container and ignition of the hydrogen released. The release and ignition are videotaped. Perform a spectral analysis of the hydrogen flame to determine source of the visible light. Previous work has shown that the vehicle will be undamaged.
6. Restore the vehicle to its stock gasoline fueled form. This involves removal of the hydrogen fuel compartment and installation of a new trunk lid
7. Perform a gasoline leak accident simulation. This involves a simulated puncture of the gasoline fuel tank and ignition of the leaking gasoline. The release and ignition are videotaped. It is expected that this will destroy the vehicle.
8. Dispose of the vehicle and repair the facilities.

Fuel Leak Simulation University of Miami						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Production of Fuel Leakage and Ignition Video						
Acquisition of vehicle and preparation of site	◆					
Prep vehicle	★					
Video taping of experiments		◆				
Spectral Analysis of Hydrogen-Air Flame						
Conduct spectral analysis		◆				
FY 2001 Begins October 1, 2000						

Distributed Hydrogen Fueling Systems Analysis - Directed Technologies, Inc.

During FY '2000 DTI completed the first year of a three-year contract to evaluate additional details regarding the major fuel options for fuel cell vehicles: hydrogen, gasoline and methanol. The tasks for FY 2001 shift from the three fuel comparison to a comparison and assessment of techniques to produce hydrogen at the local fueling station – the scenario identified as the most cost-effective in previous DTI studies for the DOE and the Ford Motor Company. By producing hydrogen from natural gas at the local fleet operator's garage or local fueling station, the costs of hydrogen transportation from a large central hydrogen plant are avoided. That is, hydrogen from a large plant must be shipped by either pipeline or it must be liquefied and shipped by cryogenic tanker truck. Either option is very expensive, eliminating the economies generated by producing bulk hydrogen at a central facility. Furthermore, the distributed hydrogen production at the local fueling station permits a gradual, incremental build-up of the hydrogen infrastructure, reducing the "chicken-and-egg" investment dilemma facing fuel suppliers and auto makers. Hydrogen fueling appliances can be added where and when they are needed to match an evolving fuel cell vehicle market.

Assuming that funding is received, DTI plans on completing these tasks during FY 2001²:

Task 1: Compare Steam Methane Reforming (SMR) with Autothermal Reforming (ATR) of Natural Gas

Subtask 1-1: Analyze and compare the cost and performance of a stationary natural gas steam reformer system with a stationary natural gas autothermal reformer for the purposes of developing a low-cost, mass producible hydrogen fueling appliance.

Subtask 1-2: Estimate the cost and performance of an integrated fueling appliance including gas compression, storage and dispensing when integrated with a natural gas steam reformer.

Subtask 1-3: Estimate the cost and performance of an integrated fueling appliance including gas compression, storage and dispensing when integrated with a natural gas autothermal reformer system.

Distributed Hydrogen Fueling Systems Analysis Directed Technologies, Inc.						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Compare SMR with ATR						
SMR cost and performance			◆			
ART cost and performance				◆		
Fueling appliance cost and performance with SMR					◆	
Fueling appliance cost and performance with ART					★	
Compare H₂ Gas Purification Option					◆	

FY 2001 Begins October 1, 2000

²These tasks were modified relative to the initial tasks in our contract in consultation with Dr. Sig Gronich, the Hydrogen Program Manager, during the course of the first year's analysis activities.

Task 2: Compare Various Hydrogen Gas Purification Techniques

Analyze and compare the cost and performance of various gas cleanup systems suitable for a hydrogen fueling appliance including:

- pressure swing adsorption (PSA)
- hydrogen-permeable membranes preferential oxidation (PROX) systems polymer membranes

Strategic Response to Scenario Planning – National Renewable Energy Laboratory

This effort stems from HTAP's recommendation in its Report to Congress that the "Hydrogen Program host vision setting/scenario development exercises, including workshops" to "develop compelling visions and scenarios of a hydrogen energy future. . . [that will] advance the concept of hydrogen energy to senior DOE management, the Congress, and the public" (Sec. 3.1). The scenarios will help to link HTAP's overarching vision and the Program's RD&D project portfolio by providing a "rationale" for the Program.

Scenarios are tools to provide a context to explore a chosen topic. In this effort, the topic is the DOE Hydrogen Program's RD&D portfolio. The purpose is to apply a scenario planning process to develop a long-term rationale for hydrogen RD&D sponsored by the DOE Hydrogen Program. The scenarios will be used by HTAP to educate government policymakers and Congress, and to engage and excite the public about the future of hydrogen. For instance, the stories will be used in preparing suggested topics for the reauthorization of the legislation and in the explanation of the need for a complex diversified program throughout government.

The report by the World Business Council for Sustainable Development (WBCSD) identifies three phases in scenario planning: Global Scenarios; Focused Scenarios; and Strategy Development. Given limitations of time and funding, NREL proposes that an abridged Phase 1 be conducted by gleaning what it needs from available scenarios, such as those developed by the WBCSD, the Intergovernmental Panel on Climate Change (IPCC), and the World Energy Council (WEC) under multi-year, multi-million dollar projects. NREL further proposes that the HTAP Scenario Planning Committee's effort should concentrate on Phase 2, Focused Scenarios. In the WBCSD process, the focused scenarios are specific to a corporation and set the context for business strategy. For HTAP, the focused scenarios will be energy and hydrogen-specific and will set the context for strategic planning by the Hydrogen Program.

Task 1: Strategic Response Workshop

After adoption and transmittal of the scenarios, HTAP, DOE, NREL, and other national laboratories will convene a workshop to develop strategic responses to each of the HTAP scenarios. Given the futures identified in the scenarios, the participants will develop strategies for the DOE to achieve the overarching HTAP vision of hydrogen being one of two principal energy carriers in the 21st Century. The strategic responses will focus on opportunities for hydrogen, key barriers, strengths and weakness of the Program to seize the opportunities and overcome the barriers, and to identify RD&D needs and priorities.

Strategic Response to Scenario Planning National Renewable Energy Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Strategic Response Workshop						
Conduct workshop		◆				
Develop strategic response to scenarios				★		
FY 2001 Begins October 1, 2000						

Hydrogen Technical Analysis - Arthur D. Little Inc.

The Department of Energy has been working in a variety of areas associated with most of the hydrogen supply chain – production, storage, and utilization. However, one area that consistently receives only moderate attention throughout the hydrogen community is the purification of the hydrogen produced. While some efforts are being expended on absorption systems and certain membrane systems at the fundamental level, very little attention has been paid to the requirements for integration into small-scale hydrogen production systems and the effect they have on overall system efficiency, complexity, and cost. This is of concern as many of the projected uses of this hydrogen (e.g. fuel cells) have rather stringent requirements for hydrogen purity. Nevertheless, no hydrogen infrastructure can be built without the technology.

Given the importance of hydrogen purification technologies, and in the interest of ensuring a balanced approach promoting the development of technologies and policies that encourage the widespread use of hydrogen, Arthur D. Little will focus the effort in this study on the review of hydrogen purification technologies not currently funded by DOE. Specifically, they will investigate what hydrogen purification technologies are being developed (or should be developed) and how they fit with the existing and emerging production technologies on one hand and with existing and emerging storage and end-use technologies on the other.

Arthur D. Little will review three key types of hydrogen purification technologies and assess them in the context of different raw hydrogen production technologies (small-scale SMR, ATR, and biological production), storage/transportation technologies (pressurized tanks, physical media, hydrogen grid), and utilization technologies (IC engines, fuel cell systems). The three key types of small-scale purification investigated here will be PSA, membranes, and other. The most promising non-DOE funded technology from each type will be selected and a detailed analysis will be performed on each. The detailed analysis will require the development of a screening model that will characterize the overall system performance and cost. The model will include a description of the production, storage/transportation, and utilization modules based on in-house information (and DOE input as appropriate), into which the purification modules will be integrated. Based on the results of the model analysis and discussions with purification technology developers, they will prepare three separate white papers and a final report summarizing their results.

Task 2: Small-scale PSA Investigation

Although PSA systems are now the technology of choice for hydrogen purification in large-scale systems, they are not generally optimized for small-scale operation. In fact, PSAs used in small-scale systems represent significant losses (of up to 20% of the hydrogen) which could very well eliminate any energy efficiency benefits otherwise applicable to a hydrogen fuel chain. Arthur D. Little will investigate the opportunities for small-scale PSAs in interviews with key PSA system developers. Key factors in the assessment of small-scale PSAs will be:

- Efficiency (possibility for recycle, system integration)
- Operating pressure
- Impact of impurities on hydrogen recovery
- Advanced sorbent materials
- Use of PSA as a pre-purification step, not to remove the last ppm level impurities
- System controls

Task 3: Membranes Investigation

The research team will investigate recent developments in membrane technology for hydrogen purification. Recognizing DOE's efforts in so-gel-based membranes, and certain composite hydride membranes, they will focus on the most promising other membrane technology. Membrane technologies considered could include:

- Polymeric hydrogen transport membranes
- Polymeric facilitated transport membranes (impurity is permeate)
- Ceramic membranes
- Composite dense-metal membranes

Of all these technologies, one will be selected for detailed analysis.

Hydrogen Technology Analysis Arthur D. Little, Inc.						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Small-scale PSA Detailed Investigation						
Develop draft criteria model		◆				
Complete technology analysis			◆			
Membrane Detailed Investigation						
Develop draft criteria model		◆				
Complete technology analysis			◆			
Alternative Purification Technology Detailed Investigation						
Develop draft screening model		◆				
Complete technology analysis			◆			
Preparation of Final Reports						
Draft report to DOE			★			
Final report and white paper to DOE				◆		

FY 2001 Begins October 1, 2000

Task 4: Alternative Purification Technology Investigation

An investigation of other purification technologies that have been proposed will be conducted. Some of these technologies are better suited for bulk separation, while others are better suited for removal of trace elements. The technologies to be considered will include:

- Hydride-bed based separation systems (e.g. impurity-tolerant hydrides are used in a swing-bed to provide ultra-high-selectivity separation)
- Slurry-based hydride systems
- Hydrate-based removal of gases (E.g. CO₂ CH₄)
- Small-scale liquefaction and distillation (e.g. using small-scale ultra-coolers now becoming available)
- Chromatographic separation

Of all these technologies, one will be selected for detailed analysis.

Task 5: Preparation of Final Reports

In this task the results from each technology analysis will be summarized in a white paper (one for each technology), and provide a presentation-style summary report. The analysis results will include a characterization of the technology (performance, maturity, risks, cost), comparison to conventional methods, potential niche markets/applications, and recommendations for future development. They will provide a draft of each of these reports to DOE for review and comment well ahead of the end of their contract, in order to ensure opportunity for feedback. The submittal of these draft documents will be the critical milestone in their schedule. Finally, three white paper final drafts and a final report summarizing the results will be submitted to DOE.

Billings Fuel Cell Project – Big Sky Economic Development

Information not available at time of printing.

Technoeconomic Analysis of Area 2 Hydrogen Production - Florida Solar Energy Center (FSEC)

The aim of this research is to assess the issues of cost, safety, performance, environmental impact, and barriers to commercialization associated with the production of hydrogen by several technology areas (*i.e.* Area 2) not presently funded by the U.S. DOE Hydrogen Program. The hydrogen rich feedstocks to be considered are: water, natural gas (methane and hydrogen sulfide) and ammonia, and the three technology areas to be analyzed are:

- Solar thermochemical cycles for splitting water
- Thermochemical cycles/processes for splitting hydrogen sulfide (H_2S) and methane
- Catalyzed micro-reformer for splitting ammonia

The ultimate objectives of this analysis are; the comparison of the technology areas 1 & 2 to other hydrogen production schemes including steam reformation of natural gas, the determination of the feasibility of the technology area 3 as a means of supplying H_2 to vehicular and small-scale fuel cell systems and the comparison of the technology area 3 to conventional fuels with respect to storage, safety, etc.

Task 1: Analysis of the Solar Thermochemical Cycles for Splitting Water

The aim of this task is to assess the state-of-the-technology for hydrogen production based on thermochemical water splitting cycles (TCWSCs) can be integrated with a suitable solar heat source. TCWSCs that will be analyzed include, but not limited to the following cycles:

- Bowman-Westinghouse process for direct electrolysis of sulfur dioxide and water
- Norman-General Atomics cycle involving iodine and thermal decomposition of HI
- Bowman-JRC process involving bromine and electrolysis of HBr
- SynMet process for solar co-production of zinc and hydrogen rich gas
- UT-3 cycle

FSEC will review and fully assess all prospective TCWSCs with respect to the Area 2 requirements (*i.e.* process efficiency, cost, safety, ease of implementation and impact of the latest materials innovations). Standard cost analysis methodology will be employed and if needed, a suitable chemical process simulator will also be selected and used. Deliverables for Task 1 analysis include a comprehensive assessment and compilation of the cost-benefits of prospective processes for solar thermochemical splitting of water for H_2 production.

Task 2: Analysis of Thermochemical Processes for Splitting H_2S and H_2S /Methane

Natural gas (NG), in the form of methane (CH_4)/hydrogen sulfide (H_2S) mixture is a desirable feedstock if it can be used to produce hydrogen without releasing greenhouse and/or acid gases into the atmosphere. Traditionally, for natural gas processing, H_2S is viewed as a gaseous pollutant in NG requiring treatment and removal. Presently, H_2S produced from the hydrodesulfurization process is fed into the Claus reactor and converted into elemental sulfur and water. Clearly, it would be advantageous to perform H_2S conversion in a manner so as to recover and recycle its hydrogen content. Many chemical processes have been devised for this purpose. In this task, FSEC will revisit and analyze (from the perspective of cost, performance, safety and environmental impact) prospective processes for H_2S conversion to hydrogen without emission of the greenhouse gases.

FSEC will analyze the state-of-the-technology for the conversion of H_2S and H_2S /methane mixtures as feedstocks for thermochemical production of hydrogen. Deliverables for Task 2 analysis include a comprehensive assessment and compilation of the cost-benefits of prospective processes for thermochemical splitting of NG (CH_4/H_2S mixed gas) for hydrogen production.

Task 3: Analysis of the Catalyzed Micro-Reformer for Splitting Ammonia

The main objective of this task is to revisit the present status of the technology for CO_x -free synthesis and dissociation of ammonia for the hydrogen production and storage and use on-board vehicles. FSEC will perform a systematic analysis of the pros and cons of employing NH_3 dissociation reactor for on-demand H_2 production and delivery. The analysis includes a comprehensive assessment and compilation of the cost-benefits of prospective systems for thermochemical splitting of NH_3 and production and delivery of H_2 suitable for use with mobile as well as stationary fuel cell applications.

Technoeconomic Analysis of Area 2 Hydrogen Production Florida Solar Energy Center

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Inventory TCESCs of Value to Solar Interface						
Collect and compile process relevant data			◆			
Analyze data for performance and energy efficiency				◆		
Collect and compile cost data				◆		
Analyze data for cost effectiveness					◆	
Prepare task 1 report					◆	
Inventory TCCs for Splitting Natural Gas						
Collect and compile process relevant data			◆			
Analyze data for performance and energy efficiency			◆			
Collect and compile cost data				◆		
Analyze data for cost effectiveness				◆		
Prepare task 2 report					◆	
Catalyzed Micro-Reformer for Ammonia Splitting						
Compile database of processes for ammonia splitting		◆				
Analyze data for performance and fuel cell interface			◆			
Collect and analyze cost data				◆		
Prepare task 3 and final report					◆	★

FY 2001 Begins October 1, 2000

Table 3.7 Technology Transfer Projects		
Goal: Develop informed constituencies in the industrial and public sectors as part of a strategy to accelerate the commercialization of renewable hydrogen technologies		
Category	Project	Research
<i>Technology Transfer Activities</i>	Hydrogen Technical Analysis on Matters Being Considered by the International Energy Agency	Longitude 122 West Inc.
	Technical Analysis of Currently Funded Projects	Energetics, Inc.
	HTAP Coordination	National Renewable Energy Laboratory
	Education and Outreach Activities	National Hydrogen Association
	Outreach Activities	Sentech, Incorporated
	Comprehensive Summary of Hydrogen R&D Technologies – Storage	Energetics, Inc.
	Inventory Gap Analysis of Federally-funded Hydrogen R&D	National Renewable Energy Laboratory
	Outreach – Hydrogen Film	TBD
	Codes and Standards Activities	National Hydrogen Association

TECHNOLOGY TRANSFER

Hydrogen Technical Analysis on Matters Being Considered by the International Energy Agency – Longitude 122 West, Inc.

The U.S. Department of Energy participates in various activities of the International Energy Agency (IEA) through an Implementing Agreement and its Annexes. Hydrogen Agreement Annex 13, "Design and Optimization of Integrated Systems," calls for the U.S. to participate in three integrated system teams. The three teams and their projects are:

- Remote Power Systems
- Home/Residential Systems
- Transportation Applications.

Task 1: Annex 13 Participation and Independent Analysis

Longitude 122 West serves as U.S. Team leader for Annex 13 activities. The work involves coordinating with the three integrated system teams, participating in strategy development, and performing independent hydrogen system analysis. The goal of the analysis is to provide independent modeling and assessment, especially of capital and operating costs, for the integrated systems.

The current emphasis is on spreadsheet modeling, to make comparisons between system configurations and technologies easier. Other factors being considered are efficiency and environmental impact. Various combinations of renewable generation, hydrogen production, storage and utilization are being compared with conventional technologies. A range of sizes is under consideration.

In addition, Longitude 122 West attends expert meetings and interacts with the IEA Operating Agent at NREL. In FY2001, the spring expert meeting is tentatively planned for Scandinavia; the fall meeting is tentatively planned for Japan. Presentations at two technical meetings in the U.S. are also planned.

Hydrogen Technical Analysis on Matters Being Considered by IEA Longitude 122 West, Inc.

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Independent Analysis and Annex 13 Participation						
Attend Annex 13 Spring Experts Meeting				◆		
Attend Annex 13 Fall Experts Meetings	◆				◆	
Technical analysis and cost modeling					★	
Final Report						◆

FY 2001 Begins October 1, 2000

Technical Analysis of Currently Funded Projects – Energetics, Incorporated

Energetics, Incorporated is analyzing on-going hydrogen research and development (R&D) projects funded by the Department of Energy (DOE) Hydrogen Program. This project involves analyses that are similar to those that Energetics has performed over the past four years and is based on the premise that R&D projects may best be understood by visiting the project location. On-site visits and accompanying discussions with Principal Investigators (PI) and members of his/her team, are of great value both to the DOE Hydrogen Program and to the hydrogen community at large.

Once a project is chosen for technical assessment, a literature review is performed on the subject project. This includes a review of the last two or three years of Annual Operating Plan (AOP) submittals, monthly reports, the Annual Peer Review paper, published reviewers' consensus comments from the past few years, the PI's journal publications, and journal publications on the same or similar topics by other researchers.

Following completion of the literature review, each project's PI is then contacted and an on-site visit arranged. A set of topic questions or discussion points is drafted, based on the literature review, and sent to the PI one to two weeks prior to the visit. The scope of questions varies depending on the project, but includes detailed technical discussion points that will reveal fundamental scientific and engineering issues, as well as those related to economic, feasibility, need, and so forth.

During the site visit a tour is requested, preferably with a demonstration of the experimental process(es) as well as a presentation by the PI on the project and its current status. The major portion of the visit includes discussions based on the topic questions as well as on any other issues which may result from the tour, demonstration, and PI presentation.

Following each meeting, Energetics writes a comprehensive report that discusses the project in detail. The report, geared to the hydrogen stakeholder, includes information on the project's goals, status, feasibility, need and likelihood of success.

Energetics' current project was commenced late in FY 2000, and one site visit was held during the fourth quarter of FY 2000. Nine additional site visits are scheduled for the first three quarters of FY 2001. If funding is available, site visit analyses will continue through the fourth quarter of FY 2001, and beyond.

Technical Analysis of Currently Funded Projects Energetics, Incorporated						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Complete first evaluation	◆					
Complete fifth evaluation			◆			
Complete 10 th evaluation				◆		
Annual Report					★	
FY 2001 Begins October 1, 2000						

HTAP Coordination – National Renewable Energy Laboratory

The Hydrogen Technical Advisory Panel (HTAP) was authorized by the Matsunaga Act of 1992 and reauthorized by the Hydrogen Future Act of 1996. The Panel serves in an advisory capacity to the Secretary of Energy, providing insight into research and development requirements for the transition to a hydrogen economy.

Two HTAP meetings per year are held, with one generally held in conjunction with the National Hydrogen Association's Annual Meeting (in the Washington, DC area in the spring). The second meeting is held in different locations to increase the accessibility of the Panel to the general public. The panel also holds special international discussions at appropriate international meetings, such as the World Hydrogen Energy Conference and the HyForum conference.

In addition to these full-panel meetings, a number of committees have been formed to develop more detailed information on specific topics of interest to the Panel and DOE. The committees meet once per year, or as necessary.

Task 1: Logistic Support

NREL provides logistic support for the coordination of the meetings, and also provides technical and clerical assistance as necessary. This includes reimbursing HTAP members and certain invited guests for their travel expenses.

Task 2: HTAP Meeting Minutes

NREL provides a report of the complete minutes and a condensed report to the DOE Designated Federal Official, as required by advisory panel regulation.

HTAP Coordination National Renewable Energy Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Logistic Support						
HTAP meeting arrangements completed	◆		◆		◆	
HTAP Meeting Minutes						
Condensed report and complete minutes sent to DOE		★		◆		◆

FY 2001 Begins October 1, 2000

Education and Outreach Activities – National Hydrogen Association

The National Hydrogen Association (NHA) looks to foster the development of hydrogen technologies and commercial applications and to promote the transition of hydrogen in the energy field. In order to facilitate hydrogen's acceptance in the public arena, the NHA will conduct outreach activities to educate and make the public aware of hydrogen's potential.

Task 1: NHA Information Exchange

The NHA will continue to analyze current domestic and international hydrogen technology development and devise a timely information exchange method between the hydrogen industry and DOE to provide current information on technology research and development. The NHA will disseminate this information to the hydrogen industry, utilities, project developers, and state and local officials through various means, such as publications, workshops, and the Internet. Development of information on potential applications of hydrogen technologies and creating technical and non-technical materials that describe research and development activities are also included in this task.

Task 2: Hydrogen Joint Working Group Outreach

The mission of the Joint Working Group of Hydrogen Association of the Americas and Pacific Rim (JWG) is to foster the use of hydrogen in member countries by sharing project information, providing a forum to present joint projects, supporting education about hydrogen, assisting in the removal of barriers to hydrogen use and meetings to assess the state of hydrogen technologies. The JWG plans and identifies tasks to be accomplished and establishes committees to oversee various activities. The chair is responsible for oversight of that task, monitors performance and reports to the JWG. Representatives from industry, government and academia from member countries may serve on these committees.

Education and Outreach Activities National Hydrogen Association						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
NHA Information Exchange						
Quarterly publication of H2 Digest/NHA News	◆	◆	◆	◆	◆	◆
Track and report on Nevada Refueling Station, CFCP		◆		◆		
University of California at Riverside Hydrogen Bus Project					★	
Deliver final technical report						
Hydrogen Joint Working Group Outreach						
Development of program plan and budget				◆		
Charter approved by membership				◆		
Conduct first of official Joint Working Group Meetings				★		
Prepare a technical report on activities						◆
Conduct a developmental meeting			◆			
Annual U.S. Hydrogen Meetings						
Conduct the 12th Annual U.S. Hydrogen Meeting			★			
Mail proceedings				◆		
FY 2001 Begins October 1, 2000						

Task 3: Annual U.S. Hydrogen Meetings

NHA will hold annual U.S. Hydrogen Meetings to increase the understanding of hydrogen energy systems and promote a forum for information exchange and acceptance of hydrogen technologies. The 12th Annual Meeting will be held March 6 – 8, 2001 in Washington, D.C. NHA will also begin to prepare for the 13th Annual Meeting to be held in FY 2002.

Outreach Activities – Sentech, Incorporated

In late FY 2000 SENTECH, Incorporated (SENTECH) initiated two contracts focused on conducting Outreach and Communication activities for the Hydrogen Program. The first task will focus on information exchange. The second task is a three-year cooperative agreement award with the Department of Energy (DOE), Golden Field Office for technical analysis. SENTECH activities, as guided by these two tasks, will help to develop the communication tools necessary to effectively convey to multiple audiences the merits of hydrogen energy systems, their challenges, and their place in a sustainable energy economy.

The activities being pursued by SENTECH will compliment the research and development work funded by the DOE by presenting the technical achievements and validations of hydrogen energy technologies to non-traditional audiences. They will also raise the visibility of DOE's Hydrogen Program within these new audiences. The ultimate benefit of the information dissemination activities will be to break the perceptual barriers - that hydrogen is unsafe, uneconomic, and of little benefit - commonly held by the uninformed. Additionally, the educational forum will help further DOE's commitment to "helping educate our nation's next generation of scientists, engineers, technicians, and educators."

Task 1 (Oakland): Information Dissemination and Outreach

Subtask 1-1: Information exchange

The objective of the Information Exchange task will be to create a searchable electronic database for the Internet that provides access to information on domestic and international hydrogen energy research, development and demonstration activities. At present, there is no single source for information on international hydrogen energy activities.

The International Energy Agency (IEA) Centre for the Analysis and Dissemination of Demonstrated Energy Technologies (CADDET) has created two energy technology databases, CADDET-EE for energy efficient technologies and CADDET-RE for renewable energy technologies. Hydrogen energy technologies are excluded from these databases because they are perceived as not yet commercially available and there is uncertainty about where hydrogen would fit, particularly since today most hydrogen is produced primarily from non-renewable natural gas. However, several hydrogen energy technologies are on the verge of commercialization and many others are in the later stages of research and development. This database will include market information and the identities of technology developers and end-users. As is the intent with the CADDET databases, the sharing of project information may lead to the formation of new national and international collaborations.

Subtask 1-2: Implementation

SENTECH staff will work with the HTAP Chairman, Mr. David Nahmias, and HTAPs Designated Federal Official, Mr. Neil Rossmiessl to identify specific tasks to assist HTAP in meeting its fiscal year 2001 planned activities and responsibilities in support of three specific HTAP themes: Scenario Planning, Fuel Choice, and Interagency Coordination.

Task 2 (Golden Field Office): Technical Analysis

Subtask 2-1: Information analysis for communication brochures

SENTECH will produce and distribute two glossy brochures that target the on-site distributed generation and public transit markets for hydrogen energy technologies. These markets represent two near-term applications for hydrogen. The brochures will answer the questions of safety, economics, and benefits by

presenting examples of successful applications of hydrogen. The brochures will be distributed at two relevant technical conferences and through traditional distribution channels.

Subtask 2-2: Industry meeting, analysis, and assessment

SENTECH will conduct face-to-face meetings with ten (10) companies from select industry sectors that have a stake in the development of hydrogen as an energy carrier. Presentations made to these groups will be tailored to their specific industries. Feedback will be incorporated into individual trip reports, and submitted as a deliverable.

The focus of these meetings will change direction from previous years in an effort to include more visits to industries that may not be aware of hydrogen energy, technologies, applications, and benefits. SENTECH will also target companies perceived as “on-the-fence” when it comes to making corporate commitments to hydrogen energy, as well as related industries that may play an important role in the development of the hydrogen energy infrastructure. The ultimate purpose of the meetings will be to educate and initiate a continuing dialog in the effort to promote hydrogen energy and address perceptual barriers.

Subtask 2-3: Educational forums and assessments

SENTECH will work with Mary Rose de Valladares of MRS Enterprises (a subcontractor on this work), to conduct two educational forums during the contract period. After five years of mounting successes, the SENTECH and MRS Enterprises team will overhaul the educational forums and involve the use of advanced communications technologies to reach even more schools and students.

The SENTECH and M.R.S. Enterprises team will identify and contact candidate middle schools in the Washington, DC area, present information on the forum, and down select candidate participants. One forum will be held in conjunction with the National Hydrogen Association (NHA) Annual Meeting in March 2001. Middle school science classes will be invited to the meeting location for an on-site educational forum. The other forum participants will be down selected at a later date. It is anticipated that the education forums will include hands-on activities for the students, child-safe experiments, and various stations where they can learn about hydrogen and hydrogen technologies. Additionally, it is expected that other program deliverable products will be included, such as: excerpts from the *Renewable Power* and *Hindenburg* videos, a hydrogen lecture by Jonathan Hurwitch, and a panel of experts drawn from the NHA meeting assembled for a question and answer period with the students. All teachers involved in the educational forums will be mailed materials packets including the *Mission H2* CD-ROM and accompanying *Teacher's Workbook*, and the *Clean Corridor Curriculum* to allow for an introduction to hydrogen through preparatory course work.

Outreach Activities Sentech, Inc.						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Develop and launch internet accessibility for international hydrogen energy projects				★		
Develop tracking database for interagency coordination activities				◆		
Produce two communication brochures			◆	◆		
Complete ten industry outreach meeting and analysis of results			◆			
Complete two education forums			◆	◆		
FY 2001 Begins October 1, 2000						

A Comprehensive Summary of Hydrogen R&D Technologies: Storage – Energetics, Incorporated

Energetics, Incorporated is compiling all available information concerning domestic and international hydrogen storage research and development for use by hydrogen stakeholders. The goal is that all necessary information on hydrogen storage will be available in one location. Information on these storage technologies will come from the DOE Hydrogen Program, activities from other government agencies, university and private research (where available), and international activities as determined by the International Energy Agency (IEA) Hydrogen Implementing Agreement Annexes on storage and integrated systems. The project will include a general database and three in-depth reports on key storage projects, based on site visits to three research laboratories.

The current project will be carried out in three tasks. The first will encompass compilation, sorting, and summarizing of information on storage options and development of a stakeholder database. The second task will involve site visits and development of in-depth reports. The third will involve disseminating all information via reports, Internet postings and other outreach methods.

Highlights of these tasks are described below.

Task 1: Compilation of Databases

Energetics will develop a database of information on hydrogen storage technologies R&D, obtained from both DOE- and non-DOE related sources.

Energetics will also develop a database of key hydrogen stakeholders from industry, utilities, projects developers, and state and local officials, among others. A copy of this database will also be a deliverable to DOE.

Task 2: In-depth Analyses of Hydrogen Storage Projects

Energetics will perform in-depth evaluation and analysis on three storage projects. Site visits will be made to each project location, preferably including a demonstration of the experimental set-up. Following the visits, detailed reports will be written on each project, with strengths, weaknesses, progress in reaching project goals, likely technology applications, and potential impact on hydrogen storage.

Task 3: Storage Report Development and Dissemination

Energetics will prepare a detailed, comprehensive report on the status and outlook for hydrogen storage. The report will be mailed/e-mailed widely, as well as up-loaded to the Internet.

**A Comprehensive Summary of Hydrogen R&D Technologies: Storage
Energetics, Incorporated**

Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Databases						
Complete stakeholder database	◆					
Complete storage database			★			
Site Visits						
Complete three site visits			◆			
Final Report						
Complete final report			◆			

FY 2001 Begins October 1, 2000

Inventory and Gap Analysis of Federally-Funded Hydrogen R&D – National Renewable Energy Laboratory

The objective of this project is to develop a comprehensive inventory of federally funded hydrogen energy research, development and demonstration projects. Searches of available databases will be conducted and will be used to develop a single database of hydrogen energy projects. Careful review of this database and grouping of projects based on research focus will provide a comprehensive inventory of hydrogen activities. This inventory will then be used to identify duplication of effort and gaps in the federal hydrogen portfolio.

Inventory of all federally funded hydrogen research and development is essential for minimizing duplication of effort and identifying research gaps. The Rand Corporation has developed (for the Office of Science and Technology Policy) a comprehensive annual database of ongoing research and development sponsored by the 24 federal agencies. Using the Research And Development In the United States (RADIUS) database, which compiles the submissions of all federal agencies work (down to the task level), NREL will conduct searches to identify those activities related to hydrogen energy RD&D.

While a number of agencies provide information on the funding associated with their activities in the RAND database, others do not. Furthermore, the database was not designed to provide accounting details. Independent accounting information for the USDA will be obtained through the Current Research Information System (CRIS) of the USDA-Cooperative State Research, Education, and Extension Service (CSREES). Other agencies will have to be contacted directly.

A preliminary search of the RADIUS database, consisting of 465 records possibly related to hydrogen, was completed. All of these records were reviewed. Just over 300 were identified as directly or indirectly related to hydrogen energy research and development.

Task 1: Taxonomy of Federally-funded Hydrogen RD&D

Based on searches that are carefully conducted to identify work relevant to hydrogen (performed throughout these agencies), NREL will develop a simple boxology (tiered categorization) to explain the current funding for hydrogen and to identify areas of funding per agency, as well as what distinguishes funding if topics are similar. For this boxology, Hydrogen R&D would be the top level, with the next-level boxes as Production, Purification, Storage, Utilization and Infrastructure. These five second-level subjects will be broken down further into specific areas. Supporting activities such as life cycle, integrated systems and technoeconomic analyses will also be inventoried.

Inventory Gap Analysis of Federally-funded Hydrogen R&D National Renewable Energy Laboratory						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Taxonomy of Federally-funded Hydrogen R&D						
Complete additional searches		◆				
Compile Funding Data from Agencies			◆			
Finalize Boxology and Taxonomy			◆			
Draft Report for DOE Review			★			
FY 2001 Begins October 1, 2000						

Technical experts from NREL and the Hydrogen Technical Advisory Panel, using the U.S. DOE Hydrogen Program's strategic and multiyear planning documents, will develop a taxonomy (detailed, tiered categorization) identifying needed research and development areas. The difference between current funding and that defined as "needed" will indicate the gaps in funding and areas for additional emphasis.

Outreach – Hydrogen Film – TBD

There have been countless articles, news reports, television documentaries, government reports and books written on a myriad of concerns associated with energy use, including environmental and health effects. Likewise, much has been written and broadcast about exciting new technologies to produce, transport and use energy that are sustainable, clean and more efficient.

The public is bombarded with information on these issues, some of it accurate, some inaccurate, some misleading, some contradictory, and, in the aggregate, confusing and hard for the average person to understand. Problems are presented without solutions. When solutions are presented, they are often disputed. As a result, people are baffled about what can and what should be done about:

- Global warming and resulting climate disruptions
- Depleting oil and gas resources
- Environmental damage and health effects from fossil fuels
- Conservation and energy efficiency
- International conflict over energy supplies
- Energy and the economy

A one-hour documentary will be produced to sort through these issues and offer a balanced projection on environmental, economic, technical, and political drivers and where they are likely to move us over the next fifty years. It will showcase promising new energy technologies and demonstrate how we can meet our energy needs while simulating economic growth and mitigating air pollution and global climate change.

This film is intended to be the premier program in a new series produced in association with WorldWatch Institute, for broadcast on Discover or PBS. It will be directed towards an educated audience with an interest in science and policy issues.

A Gantt chart and critical milestone are to be determined.

Codes and Standards (C&S) Activities - National Hydrogen Association (NHA)

Hydrogen plays a significant role in the world's energy economy, but this role is almost exclusively as a chemical - hydrogen is rarely used as a fuel. The use of hydrogen as a fuel in the utility and transportation sectors faces hurdles that need to be overcome in order to transition to a hydrogen energy economy. In addition to a lack of infrastructure to support the widespread distribution and use of hydrogen, there exists a persistent perception that hydrogen is unsafe. Widespread hydrogen use will require that safety be intrinsic to all processes and systems. To develop a hydrogen infrastructure that has the public's confidence in its safety and convenience, an industry consensus on safety issues is required. This includes the development of compatible standards and formats (e.g., the same couplings for dispensing the same form of fuel). Product certification protocols are also required. The development of codes and standards for the safe use of hydrogen is an essential aspect of the DOE Hydrogen Program.

The NHA has submitted a proposal to the U.S. Department of Energy through the Sandia National Laboratories, to identify and develop the standards necessary. The following objectives and projected milestones are based on the assumption that NHA will continue to be incrementally funded for each workshop.

Task 1: Codes and Standards Workshop

NHA will prepare for, conduct, and produce minutes for workshops on safety, codes and standards of hydrogen energy systems. Such workshops serve to bring industry and government experts together with guests from a variety of codes and standards bodies, for the purpose of advancing the development of codes and standards to assure safety of hydrogen energy systems. In addition, the proceedings of such workshops serve to educate government officials and hydrogen-related industries on the progress of hydrogen safety protocols.

Codes and Standards Activities National Hydrogen Association						
Task Designation/Milestone	2001					2002
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
November 2000 C&S workshop		★				
Proceedings mailed			◆			
March C&S session at annual meeting				◆		
Proceedings mailed				◆		
August 2001 C&S workshop					◆	
Proceedings mailed						◆
FY 2001 Begins October 1, 2000						

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4.0 STATUS and PLANS

4.1 National Recognition

As the Hydrogen Program has grown in size over the past several years, so has it grown in stature as seen by the year-to-year increase in the number of patents, patent applications, awards, and other forms of recognition of achievement. These merits are itemized in this section.

FY 1994

P. Weaver, and P. -C. Maness, "Photoconversion of Gasified Organic Materials into Biologically Degradable Plastics," U.S. Patent 5, 250,427, issued October 5, 1993.

Dr. P.F. Weaver and his NREL research group also have a patent pending entitled, "Photoconversion of Gasified Organic Materials into Single-Cell Protein."

C. Linkous, "Apparatus and Method for the Electrolysis of Water Employing a Sulfonated Solid Polymer Electrolyte," U.S. Patent 5,271,813, issued December 21, 1993.

Dr. Linkous also received the 1994 Distinguished Researcher Award from the University of Central Florida Centers and Institutes.

FY 1995

Midwest Research Institute's *President's Award* was presented to Dr. John Turner (NREL) for exceptional performance, 1995.

Dr. Eli Greenbaum of ORNL received the 1995 DOE Biological and Chemical Technologies Research Program Technical Achievement Award.

University of Hawaii - patent application: M.J. Antal: Catalytic Supercritical Gasification of Wet Biomass, U.S. Patent Application; Serial No. 08/414,523.

Oak Ridge National Laboratory - patent application: J. Woodward, S. Mattingly, and M. Danson "An Enzymatic Process for the Generation of Molecular Hydrogen from Glucose";

National Renewable Energy Laboratory - invention disclosure: D. Benson, Disclosure to NREL patent office on new design for chemochromic hydrogen detector;

Sandia National Laboratories - 3 patent disclosures:

- G. Thomas, "Metal alloy for hydrogen storage,"
- G. Thomas, "Process for manufacturing hydride beds," and
- G. Thomas, "Synthesis of magnesium alloys with controlled phase."

Energy Conversion Devices, Incorporated - patent application: K. Sapru et al. "Magnesium Mechanical Alloys for the Thermal Hydrogen Storage," Patent application serial number 08/363,205, filed 22 Dec. 1994.

FY 1996

Dr. M.J. Heben (NREL) was invited to perform research in solar production of carbon nanotubes in France at The Universite Montpellier II by the French Ministry of Foreign Affairs.

M. L. Ghirardi and M. Seibert (NREL) filed a Record of Invention Report (NREL No. 96-46) entitled "A Technique Based on H₂-Production Pressure to Select for Algal Mutants that Produce Hydrogen Under Aerobic Conditions", July 1996.

Dr. P.F. Weaver (NREL) filed a U.S. patent application entitled "Photoconversion of Thermally Gasified Biomass into Single-cell Protein."

Dr. Jonathan Woodward (ORNL) applied for a patent entitled "Enzymatic Method for Hydrogen Production from Glucose. U.S. patent application, esid-1833-x.

Dr. David Benson (NREL) filed a patent application A Fiber Optic Sensing Device@ (May 1996)

Dr. Benson was also recognized by the Hydrogen Technical Advisory Panel for "Ingenuity and Research Excellence in development of the fiber optic hydrogen sensor" (April 1996).

A U.S. Patent was awarded to Drs. C. Jensen and W.C. Kaska, University of Hawaii, entitled "Process for Alkane Dehydrogenation with Organometallic Catalyst," U.S. Patent 5,687,717.

Members of the Air Products and Chemicals, Inc. SER group have two patents pending:

- Nataraj, S.N., Carvill, B.T., Hufton, J.R., Mayorga, S.M., Gaffney, T.R., and Brzozowski, J.R., "Process for Operating Equilibrium Controlled Reactions," U.S. Patent Pending (1996).
- Mayorga, S. G., Golden, T. C., Gaffney, T. R., Brzozowski, J. R., and Taylor, F. W., A Carbon Dioxide Pressure Swing Adsorption Process Using Modified Alumina Adsorbents,@U. S. Patent Pending (1996).

C. Zawodzinski and M.S. Wilson, LANL, submitted a Formal Disclosure to the LANL Patent Office entitled "Stainless Steel Wire Mesh Flow Fields for Polymer Electrolyte Fuel Cells", November 1995.

The following recognition was afforded SERC's Palm Desert Project:

- The British Broadcasting Corporation's crew visited SERC and produced a clip that appeared during May 1996 on the BBC's show, *Tomorrow's World* .
- Newspaper and magazine articles: SERC's project was mentioned in numerous local, regional, national, and international newspapers. In addition, the December 1995 *Scientific American* ran an article about the Palm Desert Project.
- Demonstrations: Demonstrations of SERC's fuel cell powered PUV were conducted for the President of the AAA (American Automobile Association), commissioners of the CEC (California Energy Commission), the Chairman of the Board of CARB (the California Air Resources Board), at the Sacramento Municipal Utility District's Clean Power Day, at the Los Angeles Fleet Auto Show/Eco Expo, and at the City of Palm Desert's Clean Power Day.

Dr. Clovis Linkous (FSEC) was awarded U.S. patent #5,518,992, for "Photocatalytic Surfacing Agents for Inhibiting Algae Growth," May 21, 1996.

SNL has filed a patent disclosure entitled: "Continuous Microcellular Interstitial Media as an Immobilization Matrix,"

Energy Conversion Devices, Incorporated have filed the following patent applications:

- K. Sapru et al. "Robust Metal Hydride Hydrogen Storage System," Patent application serial number 08/569,487, filed 08 Dec. 1995.
- K. Sapru et al. "Robust Metal Hydride Hydrogen Storage System with Metal Support Structure," Patent application serial number 08/623,497, filed 03 Mar. 1996.

Dr. J. Bellan was awarded the Exceptional Service Award for Technology and Applications Programs from the Jet Propulsion Laboratory. The inscription reads: "In recognition of exceptional contribution in multiphase and reactive flows and combustion phenomena that have wide range of application in propulsion and aircraft engine design".

FY1997

Drs. M. L. Ghirardi and M. Seibert (NREL) filed a Patent Application on the invention entitled "A Technique Based on H_2 -Production Pressure to Select for Algal Mutants that Produce Hydrogen Under Aerobic Conditions", April 1997.

Dr. Michael Seibert received an NIS-IPP grant to work with a Russian group on a project that will support the Hydrogen Program's biohydrogen efforts.

Dr. Seibert also received an invitation from a Spanish Laboratory to give a seminar with travel expenses paid by the Spanish government.

Dr. Seibert's group also received a request from a Swiss National to join the group as a postdoctoral fellow at the expense of the Swiss government.

Dr. John Turner (NREL) and Dr. Rick Rocheleau (U Hawaii) were co-recipients of the HTAP second annual Hydrogen Program Research Success Story Award for work on "Photoelectrochemical Systems for the Production of Hydrogen".

Dr. David Benson (NREL), who had a patent application for his Hydrogen sensor in the FY 1996 listings, has also applied for an international patent. The patent application was issued in October 1997 as International Publication Number WO 97/37258. This is the first step in the process of obtaining international patents. Designated countries include Belgium, Switzerland, Denmark, Finland, Great Britain, Italy, Netherlands, Austria, Ireland, Spain, Australia, France, Luxembourg, Monaco, Portugal, Germany, Greece, Australia, Japan, and Canada.

Dr. George Thomas (SNL) has filed a patent disclosure concerning an immobilization method for a hydride bed.

Dr. Craig Jensen and his associates at the University of Hawaii have filed the following two patent applications on polyhydride storage complexes:

"Process for Alkane Dehydrogenation with Organometallic Catalyst." W. Kaska and C. Jensen; U.S. Patent 8,687,717 filed July 1996.

"Low Temperature Catalytic System for Chemical Storage of Hydrogen" Craig M. Jensen; U.S. Patent 8,807,123 filed February 1997.

Dr. Clovis Linkous of FSEC was awarded the Orlando Section of the American Chemical Society's Outstanding Chemist Award in December 1996

The SERC/Palm Desert Project has gained additional exposure to that which was reported in FY 1996: Articles about the project have appeared in:

- *Popular Science* (September 1996, October 1996)
- *Motorland Magazine* -a publication of the American Automobile Association (Nov/Dec 1996)
- *Wired Magazine* (October 1997)
- A video about the project has appeared on *Understanding Cars*, The Learning Channel, May, 1997

Oak Ridge National Laboratory Awards Night, "Technical Achievement Award, Invention" May 1997 to B. S. Hoffheins, R. J. Lauf, and P. H. Fleming.

F. Mitlitsky, B. Myers, and F. Magnotta, LLNL have filed an invention disclosure, "Lightweight bladder lined pressure vessels," *Disclosure and Record of Invention*, DOE Case No. IL-9722 (1995).

The Savannah River Bus Project was awarded the Federal Laboratory Consortium 1996 Southeast Regional Partnership Award

Personnel involved with the Savannah River Bus Project were awarded the "Keys to City of Augusta" by Mayor Larry Sconyers and Senator Sam Nunn (D-GA).

C. Zawodzinski and M.S. Wilson, of the LANL PEM Fuel Cell Team have submitted a patent application to the US Patent Office entitled "Stainless Steel Wire Mesh Flow Fields for Polymer Electrolyte Fuel Cells."

Drs. J. Bellan and R. S. Miller were awarded NASA Certificates of Recognition (recognition for best and most important papers within NASA) were awarded for the following publications:

- "Analysis of Reaction Products and Conversion Time in the Pyrolysis of Cellulose and Wood Particles"
- "A Generalized Biomass Pyrolysis Model Based on Superimposed Cellulose, Hemicellulose and Lignin Kinetics"
- "Tar Yield and Collection from the Pyrolysis of Large Biomass Particles"

Dr. Jonathan Woodward (ORNL) was awarded the Columbus Award for his glucose to hydrogen work

FY 1998

The ORNL Team won a Lockheed Martin Energy Research, Corp. invention award at the 1997 Awards Night.

Weaver, P.F., (NREL) "Photoconversion of Thermally Gasified Biomass into Single-cell Protein." U.S. Patent application filed and appeal defended.

A Notice of Allowance was received from the US Patent Office regarding M. L. Ghirardi and M. Seibert's Patent "Process for Selecting Oxygen Tolerant Algal Mutants that Produce H_2 under Aerobic Conditions" in July, 1998. (NREL)

A Patent Application on an invention entitled "A Chemochromic Sensor for Rapid Biohydrogen Phenotypic Screening" by M. Seibert, T. Flynn and D. Benson (NREL) was filed in May, 1998.

Fiber Optic Device for Sensing the Presence of a Gas, David K. Benson, Clemens S. Bechinger and C. Edwin Tracy, (NREL) US Patent No. 5,708,735, January 13, 1998.

NREL filed a provisional patent application on a closely related hydrogen sensor that is being successfully used by NREL bio-hydrogen researchers to facilitate the selection of hydrogen-producing mutant algae.

M.S. Wilson and C. Zawodzinski, (LANL) "Stainless Steel Wire Mesh Flow-Fields for Polymer Electrolyte Fuel Cells," Patent issued by the US Patent Office (No 5798187, Aug 25, 1998).

F. Mitlitsky, B. Myers, and F. Magnotta, (LLNL) *ALightweight bladder lined pressure vessels, @Disclosure and Record of Invention*, DOE Case No. IL-9722, U.S. Patent No. 5,798,156, August 25 (1998).

F. Mitlitsky, J.B. Truher, J.L. Kaschmitter, and N.J. Colella, (LLNL) *AFabrication of polycrystalline thin films by pulsed laser processing, @Disclosure and Record of Invention*, DOE Case No. IL-9123, U.S. Patent No. 5,714,404, February 3 (1998).

M.J. Antal, (U Hawaii) Catalytic Supercritical Gasification of Wet Biomass, U.S. Patent Application; Serial No. 08/414,523.

M.J. Antal, X. Xu, (U Hawaii) Catalytic Supercritical Gasification of Biomass Starch Pastes, U.S. Provisional Patent Application.

Craig M. Jensen, and William C. Kaska (U Hawaii) Patent 5,780,701 Process for Alkane and Alkyl Group Dehydrogenation with Organometallic Catalyst;. Issued 7/98.

Sandia National Laboratories Patent Disclosures and Status:

- Bed Immobilization Method **B** nearing completion
- Mg alloy **B** re-submitted

The Hydrogen Technical Advisory Panel (HTAP) awarded the Safety Analysis work at the University of Miami their Research Excellence Award on March 3, 1998 at the 9th Annual US Hydrogen Meeting

Savannah River Technology Center: Invention disclosure filed for membrane separation system.

ECD: Two patent applications filed:

- "Metal Hydride Storage Container with Valved Ports", filed 1/20/98
- "Self-Heating Metal Hydride Hydrogen Storage System," filed 2/13/98.

FY 1999

Massachusetts Institute of Technology:

- *Plasma Fuel Converter using High Voltage, Low Current Operation*, US patent Office application, 1999
- *Low Power Compact Plasmatron Fuel Converter*, US patent application (continuation-in-part of the above application), 1999
- MIT Paper presented at the Fall Meeting of the American Chemical Society was nominated for the Glen Award.

Lightweight Bladder Lined Pressure Vessels F. Mitlitsky, B. Myers, and F. Magnotta, (LLNL) *Disclosure and Record of Invention*, U.S. Patent No. 5,798,156, August 25 (1998).

Fabrication of Polycrystalline Thin Films by Pulsed Laser Processing, F. Mitlitsky, J.B. Truher, J.L. Kaschmitter, and N.J. Colella, (LLNL) *Disclosure and Record of Invention*, U.S. Patent No. 5,714,404, February 3 (1998).

A patent entitled "A Chemochromic Sensor for Rapid Biohydrogen Phenotypic Screening" by M. Seibert, D.K. Benson and T.M. Flynn (NREL) was filed, May 1999.

Weaver, P.F. (NREL) "Photoconversion of Thermally Gasified Biomass into Single-cell Protein." U.S. patent application filed and appeal defended.

Dr. James Weifu Lee (ORNL) received two awards in FY 1999:

- DOE Early Career Award for Scientists and Engineers
- Presidential Early Career Award for Scientists and Engineers.

Dr. Lee was honored in ceremonies at DOE headquarters and the Old Executive Office Building. The awards were presented by Secretary of Energy Bill Richardson and Presidential Science Advisor Neal Lane.

A patent application by R. J. Lauf, (ORNL) *Resistive Hydrogen Sensing Element*, was filed May 10, 1999.

A patent application was filed for Dr. Peter Van Blarigan (SNL) *Free Piston Engine*.

Peter Van Blarigan, Sandia National Laboratory 1998 Harry Lee Van Horning Memorial Award. This was awarded by an SAE board of award in October 1999 for the single most outstanding technical contribution to SAE for 1998 in the fields of engines, fuels and combustion.

Savannah River Technology Center: Patent was awarded on composite metal hydride materials.

M.J. Antal (U Ha) Catalytic Supercritical Gasification of Wet Biomass, U.S. Patent Application; Serial No. 08/414,523.

1999 Research Success Story Award, presented to Craig M. Jensen (U Hawaii) by the US Department of Energy Hydrogen Program Technical Advisory Panel, April 6, 1999.

Craig M. Jensen and Ragaiy A. Zidan (U Hawaii) *Novel Hydrogen Storage Materials and Method of Making by Dry Homogenation* (provisional patent filed 8/98); (full patent filed, 5/99).

M. S. Wilson (LANL) "Fuel Cell Membrane Humidification," US Patent No. 5,952,119. Sept. 14, 1999.

Sapru, Krishna; Ming, Lu; Ramachandran, Subramanian, (ECD) US Patent Number 5916381 A Magnesium Mechanical Alloys for Thermal Storage @ Aug 29, 1999

J. Woodward, and S.M. Mattingly, (ORNL) "Method for the Enzymatic Production of Hydrogen" U.S. Patent 5,942,424 Aug 24, 1999.

A provisional patent application entitled A Hydrogen Production Using Hydrogenase-Containing Oxygenic Photosynthetic Organisms @ by A. Melis, L. Zhang, J.R. Benemann, M. Forestier, M. Ghirardi and M. Seibert (U California, Berkeley and NREL) was filed on Dec. 28, 1999.

FY 2000

S. Nataraj, R.B. Moore and S.L. Russek, (Air Products and Chemicals) U.S. Patent 6048472, April 2000, A Production of Synthesis Gas by Mixed Conducting Membranes @

S. Nataraj and S.L. Russek, (Air Products and Chemicals) U.S. Patent 6077323, June 2000, A Synthesis Gas Production by Ion Transport Membranes @

S. Nataraj and S.L. Russek, (Air Products and Chemicals) U.S. Patent 6110979, August 2000, A Utilization of Synthesis Gas Produced by Mixed Conducting Membranes @

S. Nataraj, P.N. Dyer, and S.L. Russek (Air Products and Chemicals) U.S. Patent 6114400, September 2000, A Syngas Production by Mixed Conducting Membranes with Integrated Conversion into Liquid Products @

M. S. Wilson and C. Zawodzinski (LANL) A Fuel Cell with Metal Screen Flow-Field," US Patent No. 6,037,072. March 14, 2000.

A. Q. Pham, P. H. Wallman, and R. S. Glass, (LLNL) A Natural Gas-Assisted Steam Electrolyzer, @ U. S. Patent No. 6,051,125 (April 18, 2000).

Peter Van Blarigan, (SNL) A Free Piston Engine @ B pending 2000 B claims accepted

Sapru, K. (ECD) A Magnesium Mechanical Alloys for Thermal Hydrogen Storage @ US Patent No. 6,103,024, August 15, 2000

Sapru, K. (ECD) A Self-Heating Metal-Hydride Hydrogen Storage System @ US Patent No. 6,099,811, August 8, 2000

Sapru, K. (ECD) A Magnesium Mechanical Alloys For Thermal Hydrogen Storage @ US Patent Number 5,976,276, November 2, 1999

Bhandari and Baum, A Hydrogen Sensor Utilizing Rare Earth Metal Thin Film Detection Element @ US Patent Number 6,006,582, December, 1999.

Craig M. Jensen, U Hawaii, A Hydrogen Storage @ US patent # 6,074,447; issued 6/13/00.

N. Muradov (FSEC), A Thermocatalytic Process for CO₂-free Production of Hydrogen and Carbon from Hydrocarbon Fuels @ U.S. Patent Application, No. 60/194828, filed 04/05/2000

N. Muradov (FSEC), **A**Portable Hydrogen Generator[®], U.S. Patent Application, No. 60/203370, filed 05/10/2000

NREL Record of Invention IR 00-34, **A**Solar Thermal Aerosol Flow Reaction Process,[®] Alan Weimer, Jaimee Dahl, Joseph Tamburini, Allan Lewandowski, J. Roland Pitts, Carl Bingham NREL and U Colorado) UTC File No. 10058; SN 60/203, 186. Submitted as a provisional patent to the U.S. Patent Office, May 8, 2000.

The 2000 HTAP Research Success Story Award was presented to M.J. Heben for NREL's work in hydrogen storage using carbon nanotubes.

A.C. Dillon, T. Gennett, and M.J. Heben, (NREL), ROI #99-22 "Pure Single-Wall Carbon Nanotubes", was converted into a full Patent Application on 8/10/00.

A.C. Dillon, T. Gennett, J.L. and M.J. Heben (NREL) ROI #99-44 "Cutting of Single-Wall Carbon Nanotubes for Hydrogen Storage or Superbundle Formation", was filed as a Provisional Patent Application on 1/19/00.

A.C. Dillon, T. Gennett, J.L. and M.J. Heben. (NREL) ROI #00-44 "Single-Wall Carbon Nanotubes for Metal-Hydride Assisted Hydrogen Storage or Superbundle Formation", was filed on 7/7/00:

Weaver, P.F. (NREL) "Photoconversion of Organic Materials into Single-cell Protein." U.S. patent allowed. NREL IR Number 90-40FWC, serial number 07/959,519.

M. Seibert (NREL) was elected Fellow of the American Association for the Advancement of Science.

SunLine Transit Agency won the 1999 Governor's Environmental and Economic Leadership Award.

Sandia National Laboratory:

- Patent No. 5,866,623 awarded **B** Method for immobilizing particulate material in packed beds.
- Patent No. 5,895,518 awarded **B** Synthesis of alloys with controlled phase structure.
- New disclosure submitted on bed assembly, G. Cook Story and R. Baldonado.

4.2 FY 2000 Major Accomplishments

Production

Fossil-Based Production

Hydrogen Manufacturing Using Plasma Reformers B Massachusetts Institute of Technology

- A new plasma reformer was developed that promises significantly reduced overall specific energy consumption and operation at greatly decreased electrical power. It is based on nonthermal plasma technology, and operates at low current (and correspondingly higher voltage). Low current operation virtually eliminates the problem of electrode erosion with the DC arc plasmatron. The low power plasmatron can also be effectively used for applications requiring much lower hydrogen production rates. The low power plasmatron was preliminarily tested with diesel and with methane with spectacular results. The plasmatron specific energy consumption has been decreased to 3 MJ/kg H₂, without the use of heat regeneration. The electrical power in the plasmatron has been reduced to as low as 100W.
- A plasmatron reformer with a catalyst has been tested with steam addition. The CO content of the reformat has been decreased to 2% in the case of natural gas reforming, and to about 5% in the case of diesel fuel reforming.
- A cost analysis of the system showed even under conservative assumptions the cost of hydrogen could be as low as \$7-\$8/MMBTU.

Thermal Dissociation of Methane Using a Solar-Coupled Aerosol Flow Reactor- NREL/University of Colorado

- A solar-thermal aerosol flow reactor was constructed, installed and tested at the High-Flux Solar Furnace HFSF at NREL. Proof-of-concept experiments were successfully carried out for the dissociation of methane to produce hydrogen and carbon black..
- Approximately 90% dissociation of methane was achieved in a 25-mm diameter quartz reaction tube illuminated with a solar flux of 2400 kW/m² (or suns).

Production Of H₂ By Superadiabatic Decomposition Of Hydrogen Sulfide - Gas Technology Institute (GTI)

- Demonstrated theoretical feasibility of Hydrogen production over a wide range of operating conditions, and designed a lab-scale testing system to collect the necessary experimental data to demonstrate the technical feasibility of the process.

Thermocatalytic CO₂-Free Production of Hydrogen From Hydrocarbon Fuels - Florida Solar Energy Center

- The technical feasibility of CO₂-free production of hydrogen via thermocatalytic pyrolysis (TCP) of different hydrocarbons was demonstrated. Methane, propane and gasoline were efficiently converted into hydrogen-rich gas and carbon using selected carbon catalysts.
- Preliminary techno-economic assessment of the TCP process indicates that the thermocatalytic unit with the capacity of an average steam reforming (SR) plant would yield hydrogen at a cost of \$5.0/MMBTU (if carbon is sold at \$100/t), which is less than that from SR coupled with CO₂ sequestration

Novel Catalytic Fuel Reforming B InnovaTek, Inc.

- A thermal and process system model that was developed as a system simulator can be used to optimize the design of a micro channel reactor. The active length and inlet cross section of catalytic methanol reforming is optimized through temperature control and throughput rate for a specific catalyst.
- Hydrogen production is maximized and CO production is minimized by proper selection of 1) temperature-dependent reaction equilibria, 2) ratio of methanol to steam, and 3) catalyst activity.

Engineering Development of a Ceramic Membrane Reactor System for Converting Natural Gas to Hydrogen and Synthesis Gas for Liquid Transportation Fuels - Air Products and Chemicals, Inc.

- Air Products and partners have completed preliminary process designs on an offshore 55MMSCFD syngas ITM process, a 500 MMSCFD syngas land-based ITM process, a 0.5 MMSCFD distributed hydrogen ITM process, and a 150 MMSCFD hydrogen ITM process for producing fuel grade hydrogen.
- Developed, demonstrated, and selected for scaleup ITM materials with the characteristics and stability required for the ITM H₂ and ITM Syngas processes..

Separation and PurificationSeparation Membrane Development - Westinghouse Savannah River Technology Center

- Defined encapsulation conditions for Zr-Co type metal hydride in addition to La-Ni-Al type metal hydride.

Defect-Free Thin Film Membranes For H₂ Separation And Isolation B Sandia National Laboratories

- Synthesized CsZn₂OPO₄ films on ZnO membrane supports. (These films show significant permeabilities only to H₂ and He. *This is consistent with molecular sieving.*)
- Established collaboration with an academic partner (Dr. Martha Mitchell, New Mexico State University, Dept. of Chemical Engineering) for modeling and simulation work.

Electrolytic ProcessesPhotoelectrochemical Hydrogen Production - University of Hawaii, Manoa

- Developed and demonstrated a process to fabricate the new planar, integrated photoelectrodes. Initial testing using triple-junction a-Si cells supplied by the University of Toledo and thin-film catalyst and protective coatings developed at UH was conducted.
- Refined the new photoelectrode design to allow use of high-efficiency, low-voltage diodes such as CIGS (gallium-doped CIS).
- Completed construction of a small-scale reactor for parallel testing of up to six 1x1 photoelectrodes

Solar Photocatalytic H₂ Production from Water Using a Dual Bed Photosystem - Florida Solar Energy Center

- Established perylenes as effective oxidative water-splitting photocatalysts, and phthalocyanines as effective reductive water-splitting photocatalysts

Renewable Production

Photobiological Processes

Efficient Hydrogen Production Using Enzymes of the Pentose Phosphate Cycle -Oak Ridge National Laboratory

- The enzymatic conversion of glucose to H₂ resulted in the maximum yield (~12 mol of H₂ per mole of glucose) by using enzymes of the oxidative cyclic pentose phosphate pathway coupled to hydrogenase. Close to theoretical yields of hydrogen from sugar are now possible.

Hydrogen Production by Photosynthetic Water Splitting - Oak Ridge National Laboratory

- Developed a new static photobiological reactor that is based on the principle of partitioning of photosynthetically produced hydrogen and oxygen between the liquid phase and headspace.
- Discovered a mutant of *Chlamydomonas reinhardtii* that has a smaller antenna size than the wild-type alga. This mutant demonstrated better resistance to photoinhibition and a higher intensity for light saturation than wild-type.

Maximize Photosynthetic Efficiencies and Hydrogen Production in Microalgal Cultures - University of California, Berkeley

- Generated a library of 6,500 DNA insertional transformants.
- Identified mutants in Chl *b* biosynthesis having a significantly truncated Chl antenna size for photosystem-II but no effect on the Chl antenna size of photosystem-I. Identified an additional mutant aberrant in the down-regulation of the Chl antenna size having a conditionally truncated Chl antenna size for both PSII and PSI (termed *tlh1*). Both mutants suggest significantly greater photosynthetic solar conversion efficiencies under mass culture than their corresponding wild type counterparts.

A Cyclic Photobiological Algal Hydrogen Production System B National Renewable Energy Laboratory

- Discovered that inactivation of O₂ evolution occurs upon depletion from the growth medium of many other nutrients such as nitrogen, manganese and iron. However, the rate of inactivation is fastest when sulfur is withheld. Also observed that the inactivation is faster when it occurs in the light and in the presence of acetate.
- Designed and operated a fully automated and computerized photobioreactor test system. The system allows the simultaneous measurement of dissolved oxygen concentration, redox potential, pH, temperature, and amount of H₂ evolved in four independent reactors.

International Energy Agency and Other International Collaborations B National Renewable Energy Laboratory

- Final reports were published for the Annex 11 Integrated Systems activities: **A**Analysis Tools,@which contains the code details for each of the twenty-four component models developed under the activity and **A**Design Guidelines,@which includes recommendations for the optimization of existing hydrogen systems and new, promising, and desirable hydrogen systems.
- NREL experts and industrial partners participated in a planning workshop for the new IEA Hydrogen Agreement activity on Hydrogen Production from Carbon Containing Materials.

- Two papers and an exhibition display were produced for the Hyforum 2000 meeting in Munich, Germany. One paper presented an overview on the IEA Hydrogen Agreement and its activities. The second paper summarized the hydrogen programs of the member countries of the IEA Hydrogen Agreement (Canada, Japan, Lithuania, the Netherlands, Norway, Spain, Sweden, Switzerland and the United States).
- Two Executive Committee Meetings and six Experts Meetings were attended by NREL representatives. The Executive Committee meetings focused on revising the strategic plan and preparing for the Hyforum 2000 meeting. Increasing the membership in the IEA Hydrogen Agreement was also discussed. Iceland, Israel, Hungary, Portugal, Korea, Australia, Mexico and the United Kingdom have all expressed interest in joining the IEA Hydrogen Agreement and will be invited to Executive Committee and Experts Meetings during FY 2001.

Storage

Carbon Structures

Carbon Nanotube Materials for Hydrogen Storage - National Renewable Energy Laboratory

- Achieved a storage density of 7 weight % after charging with H_2 at room temperature and a pressure of 1 atm.
- Produced single-walled nanotubes (SWNT) by chemical vapor deposition. Growth was measured as a function of temperature and tubes grew most efficiently in a narrow temperature range. The process is amenable to scale-up. The tubes produced are different in diameter and type than those produced by laser vaporization, affording comparisons of hydrogen storage behavior.
- Determined that metal alloys can catalyze the addition of molecular hydrogen onto SWNT structures.

Metal Hydrides

Advanced Chemical Hydride Hydrogen Generation/Storage System for PEM Fuel Cell Vehicles - Thermo Power Corporation

- Demonstrated that the prototype hydrogen generator can meet the hydrogen demand of a simulated vehicle operating on the EPA highway and city driving protocols.
- Demonstrated lithium hydride slurry energy densities of 5110 Wh/kg and 3937 Wh/L. Demonstrated a hydrogen generation system with energy densities of 2492 Wh/kg and 1225 Wh/L. Energy density projections for a commercial system are 3361 Wh/kg and 1954 Wh/L.
- Produced hydride slurry in a semi-continuous process in 5 to 7 kg lots. Slurry is stable for months.

Catalytically Enhanced Hydrogen Storage Systems B University of Hawaii

- Discovered a new catalyst that facilitates the re-hydrogenation of Al and NaH to $NaAlH_4$ in less than one hour.

Hydrogen Storage Development - Sandia National Laboratories

- Completed hydrogen absorption and desorption measurements on a lab-scale bed to examine the behavior of NaAlH_4 as a hydrogen storage media. These measurements included (a) reaction heat generation, (b) volume changes in absorbed and desorbed states, (c) hydrogen purity from alkoxide catalyzed alanate, and (d) hydrogen capacity and cycling dependence.
- Solved hydrogen impurity and low hydrogen capacity problems in a lab-scale NaAlH_4 bed by using dry TiCl_3 as the catalyst. The problems had been associated with the liquid alkoxide process used to dope the material.
- Completely redesigned the hydride database website to be more powerful and user-friendly. New complex hydride and hydride applications databases were added.

Physical Storage

Vehicular Hydrogen Storage Using Lightweight Tanks - Lawrence Livermore National Laboratory

- Showed that thin, metallic coatings can effectively reduce hydrogen permeation (by at least a factor of three) across proven tank liner materials.
- Tapered rotational-molded tank liners have been proven capable of realizing the most mass-efficient Type IV compressed hydrogen tanks. Tanks suitable for vehicles with mass performance as high as 11.3% by weight hydrogen have just been proven feasible.

Advanced Thermal Hydrogen Compression - Ergenics, Inc.

- An analysis of advanced hydrogen production processes showed thermal compression to be viable for Algal (Photobiological), Biomass via Fast Pyrolysis/Steam Reforming, Photoelectrochemical Direct Conversion and PEM Electrolysis.

Utilization

Fuel Cells

Small Battery/Fuel Cell Alternative Technology Development B Los Alamos National Laboratory

- Air-Breather fuel cell stacks are now ~~officially~~ commercially available from Enable FC Corp.
- Demonstrated a miniature 1 W air-breather stack roughly the size of a 9V battery
- Showed that with the addition of a cooling fan, stack power is nearly tripled with a slight design alteration introduced by Enable.

Hydrogen Delivery System to PEM Fuel Cell - New Jersey Department of Transportation

- Showed that with the present design, the reaction can produce sufficient hydrogen to power fuel cells.

Low Cost Reversible Fuel Cell System - Technology Management, Inc.

- Showed that reversible H₂/O₂ fuel cell systems are potentially capable of energy storage round trip efficiencies of near 80%
- Showed that reversible H₂/O₂ fuel cell systems have projected life cycle costs significantly lower than lead acid batteries

Gallium Nitride Integrated Gas/Temperature Sensors for Fuel Cell System Monitoring for Hydrogen and Carbon Monoxide -Peterson Ridge, Llc

- Successfully fabricated GaN modulation-doping-semiconductor-field-effect-transistors (MODFETs) with Pt, Rh and PdAg gate metals
- Achieved low resistance electrical contacts that showed negligible drift in resistivity for 135 hours at 400°C in ambient air.

Internal Combustion EnginesInternal Combustion Engines Research and Development - Sandia National Laboratories

- Found the Sandia and Magnequench alternator designs to be of comparable configuration and predicted performance. The Sandia design appears to be more compact
- Industrial interest in the form of a CRADA with Caterpillar and custom built linear alternators supplied by Magnequench has materialized.

Hydrogen/Natural Gas Blends B NRG Technologies

- Determined that combustion chamber design has a strong effect on tradeoffs between hydrocarbon and NO_x emissions. Turbulent combustion chambers (high swirl) extend the lean limit of combustion, but increase NO_x emissions for the same equivalence ratio.
- Achieved 0.05 g/hp-hr NO_x emissions at 0.4 g/hp-hr total hydrocarbon emissions (methane).

Hydrogen SafetyInterfacial Stability of Thin Film Hydrogen Sensors B National Renewable Energy Laboratory

- Identified the most important issues for the stability of low cost hydrogen sensors:
 - Fouling of the palladium dissociation catalyst during exposure to air and contaminants.
 - Irreversible structural changes in the palladium catalyst that either destroy the structural integrity of the film resulting in a loss of material, or change the surface configuration such that dissociation of hydrogen is hindered.
 - Interfacial reactions at the palladium/metal oxide interface (for optical sensors).
 - Subtleties of the metal oxide (MO_x) structures that affect performance and stability

Integrated Micro-Machined Hydrogen Gas Sensor - ATMI, Inc.

- Successfully demonstrated the MEMS based H₂ gas sensor, showing response levels of greater than 120% to 0.25% H₂ in dry air, response times of < 0.5 s, and a dynamic range of <200 ppm of H₂ to >1% of H₂. Lifetimes were extrapolated to be greater than 1.5 years

High Efficiency Steam Electrolyzer B Lawrence Livermore National Laboratory

- Developed and improved both the anode and cathode catalysts. The new anode has a performance about 300% better than the previous anode material. The better catalyst electrodes have made it possible to reduce the electrolyzer operating temperature from 900°C to 700°C without loss of performance, better long-term stability, and a reduced methane coking problem. Under the lower operational temperature scenario, it also may be possible to operate at high pressure.
- Developed a complete fabrication process to make the electrolyzer stack components, which includes the anode support tube, the thin film electrolyte, the thin film cathode, and the interconnect.
- Designed and constructed a prototype electrolyzer system capable of producing 500 sccm hydrogen and with the potential to be operated up to 150 psi was.

Technology Validation**Renewable Hydrogen Systems**Integrated PV- Electrolysis/ Metal Hydride Hydrogen Generation and Storage System for Scooter Applications - Energy Conversion Devices, Inc

- Identified low cost renewable power in bagasse cogeneration, based on India's enormous bagasse resources. Preliminary estimate shows that electrolytic hydrogen produced by bagasse cogeneration would be cost competitive with the high gasoline price in India.
- Developed an alloy with good storage capacity, excellent cycle life and limited tolerance to moisture. Alloy was scaled-up for use as the 1st generation hydrogen storage material for the scooter. The alloy was also found to be thermodynamically suitable for integration with Proton Exchange Membrane (PEM) electrolyzer.
- Designed and constructed systems for performance evaluation and life-cycle studies of storage modules.
- Small vehicle, specifically two wheelers were identified to be the initial use of renewable hydrogen and metal hydrides

Hydrogen Production Through Electrolysis - PROTON Energy Systems

- Initiated Control Board design and development efforts; design is scheduled to be completed by the end of September.
- Investigations into renewable interfaces are underway with several suppliers.

Hydrogen Infrastructure

Filling up With Hydrogen 2000 B Stuart Energy Systems

- Built and successfully tested PFA Model 25; Demonstrated to Ford in Dearborn, Daimler-Chrysler in Auburn Hills, and to DOE at NHA meeting in Washington DC
- P3-1A fuel appliance delivered to SunLine Transit

Light, Medium Duty Fleet B NRG Technologies

NRG found that using exhaust gas recirculation (EGR) will reduce NOx to an acceptable level.

Hydrogen Reformer, Fuel Cell System, and Vehicle Refueling System B Air Products and Chemicals, Inc.

- Critical performance testing of the hydrogen generator prototype demonstrated viability of the reforming technology.

Insulated Pressure Vessels for Vehicular Hydrogen Storage B Lawrence Livermore National Laboratory

- Built 5 insulated pressure vessels of LLNL's own design. The vessel design includes vacuum super insulation and instrumentation to measure pressure, temperature and liquid level.
- Tested an insulated pressure vessel with liquid nitrogen over 100 cold cycles and 1000 pressure cycles. The cycles were alternated, running 10 pressure cycles followed by a temperature cycle. This test is expected to replicate what would happen to these vessels during operation in a hydrogen-fueled car. Cyclic testing has not resulted in damage to the pressure vessels.

Tested an insulated pressure vessel with liquid hydrogen in a fill test. No damage to the vessel resulted due to exposure at low temperature.

Remote Power

Alaska PEM Fuel Cell Validation Project B University of Alaska, Fairbanks

- Developed the control system for steam reformer; transferred software to SNL for test bench use.
- Evaluated integrated PEM system using hydrogen fuel (provided by SERC), finding a net electrical efficiency of about 45% (AC out to H2 in, LHV)

Analysis and Technology Transfer

Analysis Activities

Distributed Hydrogen Fueling Systems Analysis - Directed Technologies, Inc.

- Gasoline finding: sulfur removal from gasoline is essential to avoid poisoning the fuel cell anode. Analysis of sulfur removal costs shows that sulfur could be removed either at the refinery or onboard the vehicle at a cost of under 10 cents/gallon of gasoline equivalent. Desulfurization should not significantly deter the use of gasoline as a FCV fuel.

- Methanol finding: methanol reformed at a fueling station to produce hydrogen for FCVs would have to be delivered at cost less than \$0.25/gallon to be competitive with wholesale gasoline in an ICEV. To match the cost of hydrogen from a steam methane reformer with natural gas at \$5/MBTU, methanol would have to be delivered locally at less than \$0.46/gallon.
- Hydrogen finding: hydrogen produced by electrolysis with today's marginal electrical grid mix in the US could double greenhouse gas emissions compared to a conventional gasoline-powered vehicle.

Technology Transfer Activities

Energetics, Incorporated

- Completed six technical assessment reviews
- Completed techno-economic analysis of the PowerBall[®] hydrogen storage project
- Developed a new hydrogen stakeholder database

Florida Solar Energy Center

- Simplified the Hydrogen Risk Assessment Method by developing guidelines for predicting hydrogen concentrations caused by leaking hydrogen by measuring helium concentrations caused by leaking helium in simple enclosures (six-sided rectangular structures).
- Produced animation of vehicle fuel leakage in a residential garage. The animation compared the combustible clouds formed by leakage from the same vehicle fueled by gasoline, LPG, or hydrogen. This animation was used in the DOE video *Hydrogen: A Matter of Safety*.
- Assisted in the writing of ISO publications for ISO/TC 197/WG6 and ISO/TC 197/WG7.

4.3 Publications and Presentations

4.3.1 Research and Development

PRODUCTION

Fossil-Based Projects

Massachusetts Institute of Technology

L. Bromberg, D.R. Cohn, K. Hadidi, A. Rabinovich and N. Alexeev, APlasma Catalytic Reforming of Methane@ *Int. Journal of Hydrogen Energy* **24** (1999) 1131-1137.

L. Bromberg, D.R. Cohn, A. Rabinovich, N. Alexeev, R. Ramprasad and S. Tamhankar ASystem Optimization And Cost Analysis Of Plasma Catalytic Reforming Of Hydrocarbons@to be published, *Int. J. of Hydrogen Energy*.

Florida Solar Energy Center

N. Muradov, AOn Perspectives of CO₂-free Production of Hydrogen from Hydrocarbon Fuels for Small Scale Applications@, *Symposium on Hydrogen Production, Storage and Utilization, 1999 ACS Meeting*, New Orleans, 1999.

N. Muradov, ACompact Fuel Reformer for Mobile/Stationary Applications@, *Summit on Miniaturization of Energy, Chemical and Biomedical Systems*, Orlando, 1999.

N. Muradov, AHydrogen from Fossil Fuels without CO₂ Emissions@, in *Advances in Hydrogen Energy*, Ed. C.Gregoire Padro and F.Lau, Kluwer Academic/Plenum Publishers, New York, 2000, p.1-16.

N. Muradov, AHydrocarbon-based Systems for CO₂-free Production of Hydrogen@, *13th World Hydrogen Energy Conference*, Beijing, China, 2000, p.428-433.

N. Muradov, AThermocatalytic CO₂-free Production of Hydrogen from Hydrocarbon Fuels@, *DOE Hydrogen Program Annual Review Meeting*, San Ramon, CA, 2000.

N. Muradov, ARole of Hydrogen in Decarbonization of Fossil Fuels@, *Forum on Converting to Hydrogen Economy*, Fort Collins, CO, 2000.

Gas Technology Institute

J. Abbasian and F. S. Lau, AProduction of H₂ by Superadiabatic Decomposition of Hydrogen Sulfide,@ *Proceedings of the 2000 U.S. DOE Hydrogen Review Program Review*, (2000).

InnovaTek, Inc.

W. Lloyd Allen, Patricia M. Irving and William J. Thomson, AMicroreactor Systems For Hydrogen Generation And Oxidative Coupling Of Methane@, in *Proceedings of the 4th International Conference on Micro Reaction Technology*, AIChE Spring National Meeting, March 2000, Atlanta, GA, USA.

Patricia M. Irving and W. Lloyd Allen, "Micro Fuel Processor For Hydrogen Production" in Proceedings of the 2000 Conference on Small Fuel Cells, April 2000, sponsored by The Knowledge Foundation, Brookline MA.

NREL/University of Colorado

Alan W. Weimer, Jaimee Dahl, and Joseph Tamburini, Allan Lewandowski, Roland Pitts, Carl Bingham, and Gregory C. Glatzmaier, "Thermal Dissociation Of Methane Using A Solar Coupled Aerosol Flow Reactor", Hydrogen Program Annual Review 2000, May 9-11, 2000, San Ramon, CA.

Alan W. Weimer, Jaimee Dahl, and Joseph Tamburini, Allan Lewandowski, Roland Pitts, Carl Bingham, and Gregory C. Glatzmaier, "Thermal Dissociation Of Methane Using A Solar Coupled Aerosol Flow Reactor", to be presented at the AIChE Annual Meeting 2000, November 12-17, Westin Bonaventure/Marriott Downtown, Los Angeles, CA.

Biomass-Based Production

National Renewable Energy Laboratory

S. Czernik, R. French, C. Feik, and E. Chornet, "Production of Hydrogen from Hemicellulose-rich Fractions Generated through Steam Fractionation of Biomass", *Preprints of Symposia, Volume 44, No. 2, 217th ACS National Meeting*, March 21-25, 1999, Anaheim, CA, pp. 240-242.

M. Marquevich, S. Czernik, E. Chornet, and D. Montané, "Hydrogen from Biomass: Steam Reforming of Model Compounds of Fast-Pyrolysis Oil", *Energy & Fuels*, 1999, 13, 1160-1166.

S. Czernik, R. French, C. Feik, and E. Chornet, "Fluidized Bed Catalytic Steam reforming of Pyrolysis Oil for Production of Hydrogen", *Proceedings of the Fourth Biomass Conference of the Americas*, Oakland, CA, August 1999, Eds., R.P. Overend and E. Chornet; Elsevier Science Ltd., 1999, pp. 827-832.

L. Garcia, R. French, S. Czernik, E. Chornet, "Catalytic Steam Reforming of Bio-oils for the Production of Hydrogen; Effects of Catalyst Composition", *Applied Catalysis A: General*, 2000, 201, 225-239.

S. Czernik, R. French, C. Feik, E. Chornet, "Production of Hydrogen from Biomass by Pyrolysis/Steam Reforming", *Advances in Hydrogen Energy*, C.E. Grégoire Padró and F. Lau, eds., Kluwer Academic/Plenum Publishers, New York 2000, pp. 87-91.

Separation and Purification

Air Products and Chemicals, Inc.

P.N. Dyer, R.E. Richards and S.L. Russek, "ITM Technology for Oxygen Separation and Syngas Production", American Ceramic Soc. Ann. Meeting, Indianapolis, April 1999. (Invited Paper)

P.N. Dyer and C.M. Chen, "Engineering Development of Ceramic Membrane Reactor Systems for Converting Natural Gas to H₂ and Syngas for Liquid Transportation Fuels", U.S. DOE H₂ R&D Program Review, Denver, May 1999.

P.N. Dyer, R.E. Richards and S.L. Russek, "ITM Technology for Oxygen Separation and Syngas Production", U.S. DOE Alaska GTL Review, Anchorage, May 1999, Materials for Electrochemical Energy Conversion / Storage, Festschrift for Prof. Brian Steele, Imperial College, June 1999. (Invited Paper)

C.M. Chen and P.N. Dyer, "Engineering Development of Ceramic Membrane Reactor Systems for Converting Natural Gas to Hydrogen and Synthesis Gas for Liquid Transportation Fuels" U.S. DOE Fossil Energy Fuels Program Review, Cincinnati, September 1999.

P.N. Dyer and C.M. Chen, "ITM Technology for GTL Processing" Gas-to-Liquids Conference, IBC, London, February 2000.

P.N. Dyer and C.M. Chen, "Engineering Development of Ceramic Membrane Reactor Systems for Converting Natural Gas to H₂ and Syngas for Liquid Transportation Fuels" U.S. DOE H₂ R&D Program Review, San Ramone, May 2000.

Westinghouse Savannah River Technology Center

"Silica Embedded Metal Hydride" *J. of Alloys and Compounds*, 293-295 (1999) 446-451.

"Separation Membrane Development for Hydrogen" Topical Conference on Separations, 1999 AIChE Annual Conference, Dallas, TX November 1999.

Sandia National Laboratories

F. Bonhomme, T. M. Nenoff, "A Novel Crystalline Phase, Na₄Ga(PO₄)₂OH", *J. Solid State Chem.*, submitted, 2000.

F. Bonhomme, T. M. Nenoff, "A New Microporous Phase, Pyridine-templated gallo-phosphate", *Microporous and Mesoporous Materials*, submitted, 2000.

M. Mitchell, J. Autry, T. M. Nenoff, "Molecular Dynamics Simulations of Binary Mixtures of Methane and Hydrogen in Zeolite A and a novel Zinc Phosphate" *Molecular Simulations*, 2000, in preparation.

Electrolytic Processes

University of Hawaii, Manoa

Chin, G. P., "Characterization and Optimization of Indium-Tin Oxide (ITO) for Hydrogen Photoelectrodes" Masters Thesis in Electrical Engineering, University of Hawaii, August 2000.

L.H.Hihara, A. Iwane, S. Voss, R.E. Rocheleau, and Z.E. Zhang, "Initiation of Corrosion in Metal Substrates Coated with Plasma-Deposited Hydrogenated Amorphous Silicon Alloy Thin Films," *Corrosion Science*, December 1998.

Rocheleau, R.E., Miller, E. L., and A. Misra, "High Efficiency Photoelectrochemical Hydrogen Production using Multijunction Amorphous Silicon Photoelectrodes" *J. Energy and Fuels*, **12**, 3-10(1998).

Florida Solar Energy Center

C.A. Linkous, D.K. Slattey, and N.F. Gruhn, "Organic Pigments as Photocatalytic Agents in a Solar Water-Splitting Scheme" *Proceedings of the 13th World Hydrogen Energy Conference*, Beijing, China.

D.K. Slattey, C.A. Linkous, and N.F. Gruhn, **Photocatalytic Water-Splitting Using Organic Pigments as Semiconductors**, @ *Polymer Preprints*, American Chemical Society National Meeting, San Francisco, CA, March 28th, 2000.

C.A. Linkous, G.J. Carter, **Closed Cycle Photocatalytic Process for Decomposition of Hydrogen Sulfide to its Constituent Elements**, @ *Division of Fuel Chemistry Preprints*, American Chemical Society National Meeting, San Francisco, CA, March 27th, 2000.

C.A. Linkous and D.K. Slattey, **Development of a Dual Bed Photocatalytic Water Splitting System**, @ Annex 14 Experts Meeting on Photoelectrolytic Hydrogen Production, International Energy Agency Implementing Agreement on Hydrogen Energy, Canberra, Australia, March 14th, 2000.

G.J. Carter and C.A. Linkous, **Photocatalytic Production of Hydrogen from Hydrogen Sulfide**, @ Florida Academy of Science, Florida Institute of Technology, Melbourne, FL, March 10th, 2000.

C.A. Linkous (invited speaker) and D.K. Slattey, **Development of a Dual Bed Photocatalytic Water-Splitting System**, @ Symposium on Photoreaction Control and Photofunctional Materials, National Institute of Materials and Chemical Research, Tsukuba, Japan, March 16-17, 1999.

National Renewable Energy Laboratory

Xiaoping Gao, Shyam Kocha, Arthur J. Frank, and John A. Turner, **Photoelectrochemical Decomposition of Water Using Modified Monolithic Tandem Cells**, @ *International Journal of Hydrogen Energy*, **24**, p 319-325 (1999).

John A. Turner, **A Realizable Renewable Energy Future**, @ *Science*, **285**, p 5428, (1999).

Oscar Khaselev and John A. Turner, **Photoelectrolysis of HBr and HI using a Monolithic Combined Photoelectrochemical/PV Device**, @ *Electrochemistry and Solid State Letters*, **2**, pp 310-312, (1999).

Ashish Bansal and John A. Turner, **Suppression of Band Edge Migration at the p-GaInP₂/H₂O Interface Under Illumination via Catalysis**, @ *Journal of Physical Chemistry*, in print.

O. Khaselev, and John A. Turner, **High-Efficiency Integrated Multijunction Photovoltaic/ Electrolysis Systems for Hydrogen Production**, @ Accepted for publication in *International Journal Of Hydrogen Energy*.

J. Turner, **Direct Conversion Systems and the Efficiency of Hydrogen Production**, @ Material Research Conference, Cancun, Mexico, September 1999.

O. Khaselev and J. Turner, **Electrochemical Stability of GaN in Photoelectrochemical Systems for Water Splitting**, @ October meeting of the Electrochemical Society.

A. Bansal, J. Turner, **Chemical Modifications of III-V Surfaces for Photoelectrochemical Production of Hydrogen from Sunlight and Water**, @ October meeting of the Electrochemical Society.

J. Turner, **Advances in Hydrogen Production Technology**, @ Fall 1999 Forum of the Fuelcell Propulsion Institute, November 15, in Washington DC. (Invited)

J. Turner, **Renewable Energy Overview**, @ Navy Challenge Workshop, November 17, in Arlington VA. (Invited)

J. Turner, **A**The Sun Can be Tamed@symposium entitled, "The Hydrogen Society - Reality or Fiction", November 22 in Stockholm, Sweden. (Invited)

J. Turner, **A**Direct Conversion Systems for Hydrogen Production@November 24, Solar Energy Research Center, Dalarna University, in Borlange, Sweden. (Invited)

J. Turner, **A**Hydrogen Production via Photoelectrochemistry, November 25, Angstrom Solar Center in Uppsala, Sweden. (Invited)

J. Turner "Hydrogen Production from Solar Energy", Distinguished Seminar Series, Duquesne University, Mar 3, 2000, Pittsburgh, PA. (Invited)

J. Turner, **A**Hydrogen Production from Sunlight and Water via Photoelectrolysis@ University of Denver, Denver CO.(Invited)

J. Turner, "Hydrogen Production from Solar Energy", Stanford Linear Accelerator Center, Palo Alto, CA, May 8, 2000. (Invited)

J. Turner, A. Bansal, **A**Suppression of Band Edge Migration at the p-GaInP₂/H₂O Interface under Illumination via Catalysis@ 13th International Conference on Photochemical Conversion and Storage of Solar Energy, Snowmass, CO, August 2000.

Photobiological Processes

Oak Ridge National Laboratory

H. O'Neill and J. Woodward, **A**Nicotinamide Cofactors**B**Applications in Biotechnology,@in *Advances in Applied Biocatalysts*, ed. Badal. C. Saha, ACS Symposium Series, Washington, D.C. (in press).

J. Woodward, K.A. Cordray, R.J. Edmonston, M. Blanco-Rivera, S.M. Mattingly, and B.R. Evans, **A**Enzymatic Hydrogen Production/Conversion of Renewable Resources for Energy Production@, *Energy and Fuels* **14**, 197-201 (2000).

J. Woodward, M. Orr, K. Cordray, and E. Greenbaum, **A**Enzymatic Production of Biohydrogen,@*Nature*, **405**, 1014-1015 (2000).

J. W. Lee, L. J. Mets, and E. Greenbaum, **A**Improvement of Photosynthetic Efficiency at High Light Through Reduction of Chlorophyll Antenna Size@submitted for publication in *Photochem. Photobiol.* (2000).

J. Woodward, M. Orr, K. Cordray, and E. Greenbaum, "Efficient production of Biohydrogen from Glucose-6-Phosphate" *Nature* **405**.

N.I. Heyer, H. M. O'Neill, J. Woodward, M.J. Danson, and D.W. Hough **A**Isolation, Over-Expression, and Characterization of an extremely thermostable Glucose Dehydrogenase from *Sulfolobus solfataricus* for in vitro Hydrogen Production@*Extremophiles* (in preparation).

M. L. Ghirardi, L. Zhang, J. W. Lee, T. Flynn, M. Seibert, E. Greenbaum and A. Melis, **A**Microalgae: A Green Source of Renewable H₂,@*Trends. Biotechnol.* (in press 2000).

V. A. Boichenko, E. Greenbaum, and M. Seibert, "Hydrogen Production by Photosynthetic Microorganisms" in M. D. Archer and J. Barber (Eds.) *Photoconversion of Solar Energy: Volume III: Molecular to Global Photosynthesis*, Imperial College Press (in press, 2001).

University of California, Berkeley

Melis A, Neidhardt J and Benemann JR *ADunaliella salina* (Chlorophyta) with Small Chlorophyll Antenna Sizes Exhibit Higher Photosynthetic Productivities and Photon Use Efficiencies than Normally Pigmented Cells. *Journal of Applied Phycology* **10**: 515-525 (1999).

Melis A, Zhang L, Forestier M, Ghirardi GL and Seibert M *ASustained Photobiological Hydrogen Gas Production upon Reversible Inactivation of Oxygen Evolution in the Green Alga Chlamydomonas reinhardtii* *Plant Physiology* **122**: 127-136 (2000).

National Renewable Energy Laboratory

Maness, P.-C., and P.F. Weaver. "Evidence for Three Distinct Hydrogenase Activities in *Rhodospirillum rubrum*," in preparation for *Applied Microbiology and Biotechnology*.

Flynn, T., M.L. Ghirardi and M. Seibert.. *AI*solation of *Chlamydomonas* Mutants with Improved Oxygen Tolerance@ *Symposia, Fuels and Chemical Division, 1999 ACS Meeting*, **44** (4), 846:850. (1999).

Seibert, M., T. Flynn and M.L. Ghirardi.. "Strategies for Improving Oxygen Tolerance of Algal Hydrogen Production" *BioHydrogen* **99**, in press. (2000).

Flynn, T., M.L. Ghirardi and M. Seibert.. *AClassical Mutagenesis and Selection Approaches to Accumulate Multiple Phenotypes of O₂-Tolerance in H₂-Evolving Strains of Chlamydomonas reinhardtii*@ In preparation. (2000).

M. Seibert , invited talk, *AStrategies for Improving the Oxygen Tolerance of Algal Hydrogen Production*@at the Russian Academy of Sciences Institute of Basic Biological Problems at Pushchino in the Moscow region of Russia (October 1999).

M. Seibert invited talk, *AA* Chemochromic Sensor for Rapid Identification of Hydrogen-Producing Algal Clones@at the Electrochemical Society Meeting in Hawaii (October 1999).

M. Ghirardi "Isolation and Characterization of *Chlamydomonas reinhardtii* Mutants that Produce Hydrogen in the Presence of Oxygen", 9th Western Photosynthesis Conference, Pacific Grove, CA (January 2000).

M. Ghirardi, invited talk, *AGeneration of Algal Mutants that Produce Hydrogen in the Presence of Oxygen*@at the National Hydrogen Association (NHA) meeting in Washington D.C. (March 1999).

M. Ghirardi *ACHlamydomonas reinhardtii* Mutants that Produce Hydrogen Continuously in the Presence of Oxygen@9th International Conference on the Cell and Molecular Biology of *Chlamydomonas* in Amsterdam, The Netherlands, May 2000).

M. Forestier, *AAre there Multiple Fe-hydrogenases in the green alga Chlamydomonas reinhardtii?*@Vth International Conference on the Molecular Biology of Hydrogenases meeting in Potsdam, Germany, (August 2000).

M. Ghirardi, A Classical Genetics Approach for Generation of Green Algal Mutants that Evolve Hydrogen in the Presence of Oxygen@ VIth International Conference on the Molecular Biology of Hydrogenases meeting in Potsdam, Germany (August 2000).

Melis, A., L. Zhang, M. Forestier, M.L. Ghirardi and M. Seibert.. ASustained Photobiological Hydrogen Gas Production upon Reversible Inactivation of Oxygen Evolution in the Green Alga *Chlamydomonas reinhardtii*". *Plant Physiol.* 122, 127-135 (2000).

Ghirardi, M.L., L. Zhang, J.W. Lee, T. Flynn, M. Seibert, E. Greenbaum and A. Melis. A Microalgae: a Green Source of Renewable H₂@ *Trends Biotechnol.*, in press (2000).

M. Ghirardi, invited talk, A Reversible Two-Stage System for Sustained Algal Hydrogen Production@ at the University of Wyoming, Laramie (November 1999).

Z. Huang, A Development of a Two-Stage System for Sustained Algal Hydrogen Production@ 22nd Symposium on Biotechnology for Fuels and Chemicals, Gaitlinburg TN (May 2000).

M. Ghirardi, invited plenary lecture, Meeting A A New Algal Hydrogen-Production System@ Canadian Hydrogen Association, Quebec, Canada (May 2000).

M. Seibert, A Strategies to Develop a Sustainable Algal H₂-Production System@ 13th International Conference on Photochemical Conversion and Storage of Solar Energy, Snowmass, CO (May 2000).

M. Seibert, invited plenary speaker, A A New Direction for Algal Biohydrogen Production@ VIth International Conference on the Molecular Biology of Hydrogenases meeting in Potsdam, Germany. August 2000.

A IEA Agreement on the Production and Utilization of Hydrogen 1999 Annual Report,@ C. Elam, editor, September 2000.

A IEA Agreement on the Production and Utilization of Hydrogen,@ Brochure, C. Elam, editor, August 2000.

C. Elam (ed.), "1998 Annual Report International Energy Agency Agreement on the Production and Utilization of Hydrogen."

T. Schucan, "Case Studies of Integrated Hydrogen Energy Systems," C. Gregoire-Padró (ed.).

E. Skolnik and V. Putsche A Analysis Tools@ C. Gregoire-Padró (ed.).

M. Bracht and A. de Groot, "Design Evaluation and System Comparison Guidelines," C. Gregoire-Padró (ed.).

C. Gregoire-Padró, " Natural Gas and Hydrogen - Partners in an Energy Future," meeting paper, World Gas Conference, Nice, France, June 4-9, 2000.

N.P. Rossmeissl (drafted by C. Elam), "The International Energy Agency's Hydrogen Research and Development Activities," meeting paper, submitted to Hyforum 2000.

T. Riis (drafted by C. Elam), "National Hydrogen Programs of the IEA Member Countries," meeting paper, submitted to Hyforum 2000.

STORAGE

Carbon Structures

National Renewable Energy Laboratory

G.L. Hornyak, L. Grigorian, A.C. Dillon, T. Gennett, P.A. Parilla, K.M. Jones, and M.J. Heben, "Temperature Dependence of Single-Wall Carbon Nanotube Growth during Chemical Vapor Deposition" manuscript in preparation.

A.C. Dillon, T. Gennett, J.L. Alleman, P.A. Parilla, K.M. Jones, G.L. Hornyak and M.J. Heben, "Rapid, Room Temperature, High-Density Hydrogen Adsorption on Single-Walled Carbon Nanotubes at Atmospheric Pressure Assisted by a Metal Alloy", submitted to *Science*.

C. M. Brown, T. Yildirim, D. A. Neumann, M. J. Heben, T. Gennett, A. C. Dillon, J. L. Alleman and J. E. Fischer, "Quantum Rotation of Hydrogen in Single-Wall Carbon Nanotubes", accepted for publication in *Chemical Physics Letters*.

T. Gennett, A.C. Dillon, J.L. Alleman, K.M. Jones, F.S. Hasoon, and M.J. Heben, "Formation of Single-Wall Carbon Nanotube Superbundles" *Chemistry of Materials* **12**, 599-601 (2000).

A.C. Dillon, P.A. Parilla, J.L. Alleman, J.D. Perkins, and M.J. Heben, "Controlling Single-Wall Carbon Nanotubes Diameters with Variation in Laser Pulse Power" *Chemical Physics Letters* **316** 13-18 (2000).

A.C. Dillon, T. Gennett, K.M. Jones, J.L. Alleman, P.A. Parilla, and M.J. Heben "A Simple and Complete Purification of Single-walled Carbon Nanotube Materials" *Advanced Materials* 111354-1358 (1999).

A.C. Dillon, T. Gennett, J.L. Alleman, P.A. Parilla, and M.J. Heben "Carbon Nanotube Materials For Hydrogen Storage" *Proceedings of the 2000 U.S. DOE Hydrogen Program Review*, San Ramon, CA, May 9-11, 2000.

M.J. Heben: "Hydrogen Storage", University of Colorado, Boulder, CO, November 11, 1999.

M.J. Heben: "Carbon Nanotube Materials for Hydrogen Storage" University of Pittsburgh, Pittsburgh, PA, January 21, 2000.

M.J. Heben: "Carbon Nanotube Materials for Hydrogen Storage" Pennsylvania State University, College Station, PA, January 1, 2000.

M.J. Heben: "Hydrogen Storage in Carbon Nanotubes" International Winterschool on Electronic Properties of Novel Materials, Kirchberg, Austria, March 4-11, 2000.

M.J. Heben: "Hydrogen Storage in Carbon Nanotubes" Knowledge Foundation Meeting, New Orleans, LA, April 28, 2000.

A.C. Dillon "A Simple Purification of Single-walled Carbon Nanotube Materials", 2000 Electronic Materials Conference Symposium: Nanostructure Fabrication, Denver, CO, June 21-23, 2000.

M.J. Heben, "Carbon Materials and Hydrogen Storage" Meeting of the Experts of Annex 12 of the International Energy Agency, Davos, Switzerland. February 1-2, 2000.

Metal Hydrides

University of Hawaii

Ragaiy A. Zidan, Satoshi Takara, Allan G. Hee, and Craig M. Jensen; AHydrogen Cycling Behavior of Zirconium and Titanium-Zirconium Doped Sodium Aluminum Hydride. @ *Journal of Alloys and Compounds*, **285**, 119. (1999).

Craig M. Jensen, Ragaiy Zidan, Nathan Mariels, Allan Hee, and Chrystel Hagen; AAdvanced Titanium Doping of Sodium Aluminum Hydride: Segue to a Practical Hydrogen Storage Material? @ *International Journal of Hydrogen Energy* **24**, 461 (1999).

Fuchen Liu, Esther B. Pak, Bharat Singh, Craig M. Jensen, and Alan S. Goldman; ADehydrogenation of n-Alkanes Catalyzed by Iridium Pincer Complexes: Regioselective Formation of Alpha-Olefins. @ *Journal of the American Chemical Society*, **121**, 4086 (1999) (subject a *Chemical and Engineering News* feature article, 7/5/99).

Craig M. Jensen A Iridium PCP Pincer Complexes: Highly Active and Robust Catalysts for Novel Homogeneous Aliphatic Dehydrogenations. @ (invited feature article) *Journal of the Chemical Society, Chemical Communications* **1999**, 2443.

David Morales-Morales, Christian Grause, Kristie Kasaoko, Rocío Redón, Roger E. Cramer and Craig M. Jensen, AHighly Efficient and Regioselective Production of Trisubstituted Alkenes Through Heck Couplings Catalyzed by a Palladium Phosphinito Pincer Complex. @ *Inorganica Chimica Acta*, **300**, 958 (2000).

Shuhua Li, Michael B. Hall, Juergen Eckert, Craig M. Jensen, and Alberto Albinati ATransition Metal Polyhydride Complex. 10. Intramolecular Hydrogen Exchnage in the Octahedral Iridium (III) Dihydrogen Dihydride Complexes $\text{IrX H}_2(\text{h}^2\text{-H}_2)(\text{PR}_3)_2$ ($\text{X} = \text{Cl}, \text{Br}, \text{I}$). @ *Journal of the American Chemical Society*, **122**, 2903 (2000).

David Morales-Morales, Rocío Redón, Cathleen Yung, and Craig M. Jensen; AHigh Yield Olefination of a Wide Scope of Aryl Chlorides Catalyzed Without Additives by the Phosphinito Palladium PCP Pincer Complex: $[\text{PdCl}\{\text{C}_6\text{H}_3\text{-2,6-(OPPr}^i\text{)}_2\}]$. @ *Journal of the Chemical Society, Chemical Communications* **2000**, 1619.

David Morales-Morales, Esther B. Pak, Cathleen Yung, and Craig M. Jensen ASelective Catalytic Dehydrogenation of Linear Alkanes to Alpha Olefins by Iridium PCP Pincer Complexes Without a Hydrogen Acceptor @ *Journal of the Chemical Society, Chemical Communications* **2000**, in press.

Sandia National Laboratories

Gross, K.J. , Guthrie, S.E., Takara, S., and Thomas, G.J., AIn-situ X-Ray Diffraction Study of the Decomposition of NaAlH_4 , *J. Alloys and Compounds*, 297, (2000).

G. Sandrock and G. Thomas, AMetal Hydrides and Carbon for Hydrogen Storage: International R&D Activities under Task 12 of the IEA Hydrogen Implementing Agreement @ Proc. 9th Canadian Hydrogen Conference, Canadian Hydrogen Association, 1999, p. 94.

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